Welcome to STN International! Enter x:x

LOGINID: SSSPTA1600RXA

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NEWS X25

TERMINAL (ENTER 1, 2, 3, OR ?):2

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NEWS
                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
                 "Ask CAS" for self-help around the clock
NEWS
                 Pre-1988 INPI data added to MARPAT
         FEB 21
NEWS
                 STN AnaVist, Version 1.1, lets you share your STN AnaVist
                 visualization results
         FEB 22
                 The IPC thesaurus added to additional patent databases on STN
NEWS
                 Updates in EPFULL; IPC 8 enhancements added
NEWS
         FEB 22
      6
NEWS
      7
         FEB 27
                 New STN AnaVist pricing effective March 1, 2006
NEWS
     - 8
         MAR 03
                 Updates in PATDPA; addition of IPC 8 data without attributes
NEWS
         MAR 22
                 EMBASE is now updated on a daily basis
                 New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS 10
         APR 03
                 Bibliographic data updates resume; new IPC 8 fields and IPC
NEWS 11
         APR 03
                 thesaurus added in PCTFULL
NEWS 12
         APR 04
                 STN AnaVist $500 visualization usage credit offered
NEWS 13
         APR 12
                 LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS 14
         APR 12
                 Improved structure highlighting in FQHIT and QHIT display
                 in MARPAT
        APR 12
NEWS 15
                 Derwent World Patents Index to be reloaded and enhanced during
                 second quarter; strategies may be affected
NEWS 16
         MAY 10
                 CA/CAplus enhanced with 1900-1906 U.S. patent records
NEWS 17
         MAY 11
                 KOREAPAT updates resume
         MAY 19
NEWS 18
                 Derwent World Patents Index to be reloaded and enhanced
NEWS EXPRESS
              FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
              CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
              V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT
              http://download.cas.org/express/v8.0-Discover/
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              For general information regarding STN implementation of IPC 8
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Enter NEWS followed by the item number or name to see news on that specific topic.

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Thank you in advance for your participation.

FILE 'HOME' ENTERED AT 08:44:35 ON 24 MAY 2006

=> fil reg
COST IN U.S. DOLLARS

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
0.21
0.21

FILE 'REGISTRY' ENTERED AT 08:44:42 ON 24 MAY 2006 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2006 American Chemical Society (ACS)

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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http://www.cas.org/ONLINE/UG/regprops.html

Uploading C:\Program Files\Stnexp\Queries\QUERIES\106810021.str

chain nodes : 6 7 8 16 17 18 19 20 23 24 25 27 28 29 32 ring nodes : 1 2 3 4 5 10 11 12 13 14 15 chain bonds : 2-6 3-15 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28 8-29 10-20 11-19 12-16 13-17 14-18 ring bonds : 1-2 1-5 2-3 3-4 4-5 10-11 10-15 11-12 12-13 13-14 14-15 exact/norm bonds : 1-2 1-5 2-3 2-6 3-4 3-15 4-5 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28 8-29 10-20 11-19 12-16 13-17 14-18 normalized bonds : 10-11 10-15 11-12 12-13 13-14 14-15 isolated ring systems : containing 1 : 10 :

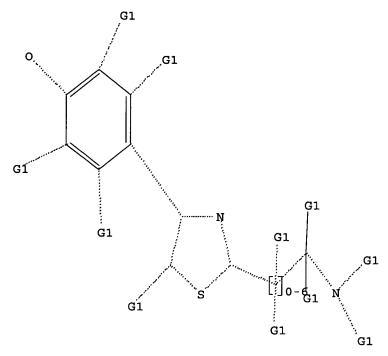
G1:C,H

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 23:CLASS 24:CLASS 25:CLASS 27:CLASS 28:CLASS 29:CLASS 32:CLASS

L1 STRUCTURE UPLOADED

=> d L1 HAS NO ANSWERS L1 STR



G1 C,H

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 08:45:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 706 TO ITERATE

100.0% PROCESSED 706 ITERATIONS 12 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

PROJECTED ITERATIONS: 12526 TO 15714

PROJECTED ANSWERS: 33 TO 447

L2 12 SEA SSS SAM L1

=> s l1 full FULL SEARCH INITIATED 08:45:11 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 14067 TO ITERATE

100.0% PROCESSED 14067 ITERATIONS 336 ANSWERS

SEARCH TIME: 00.00.02

L3 336 SEA SSS FUL L1

=> s 13 and caplus/lc

50652292 CAPLUS/LC

L4 115 L3 AND CAPLUS/LC

=> s 13 not 14

L5 221 L3 NOT L4

=> d 15 200

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L5 ANSWER 200 OF 221 REGISTRY COPYRIGHT 2006 ACS on STN
RN 642079-05-8 REGISTRY
ED Entered STN: 27 Jan 2004
C 2-Thiazoleethanamine, 4-[4-ethoxy-3,5-bis(1-methylpropyl)phenyl]- (9CI)
(CA INDEX NAME)
FS 3D CONCORD
MF C21 H32 N2 0 S
SR Chemical Catalog
Supplier: ACB Blocks Ltd
LC STN Files: CHEMCATS
```

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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LS ANSWER 210 OF 221 REGISTRY COPYRIGHT 2006 ACS on STN
RN 642078-80-6 REGISTRY
ED Entered STN: 27 Jan 2004
C 2-Thiazoleethanamine, 4-[3-(1,1-dimethylethyl)-4-(phenylmethoxy)phenyl)-
(9CI) (CA INDEX NAME)
S 3D CONCORD
MF C22 H26 N2 O S
Chemical Catalog
Supplier: ACB Blocks Ltd
LC STN Files: CHEMCATS
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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 RN ED CN

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

INDEX NAME)
3D CONCORD
C20 H22 N2 O S
Chemical Catalog
Supplier: ACB Blocks Ltd
STN Files: CHEMCATS

L5 RN ED CN (CA

FS MF SR LС

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ANSWER 216 OF 221 REGISTRY COPYRIGHT 2006 ACS on STN 642078-66-8 REGISTRY Entered STN: 27 Jan 2004 2-Thiazoleethanamine, 4-[2,5-dimethyl-4-(phenylmethoxy)phenyl)- (9CI)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ANSWER 219 OF 221 REGISTRY COPYRIGHT 2006 ACS on STN 642078-39-5 REGISTRY Entered STN: 27 Jan 2004 2-Thiazoleethanamine, 4-(4-phenoxyphenyl)- (9CI) (CA INDEX NAME) 3D CONCORD C17 H16 N2 O S Chemical Catalog Supplier: ACB Blocks Ltd STN Files: CHEMCATS

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT **

ANSWER 220 OF 221 REGISTRY COPYRIGHT 2006 ACS ON STN 64193-23-9 REGISTRY Entered STN: 27 Jan 2004
2-Thiazolethanamine, 4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME) 3D CONCORD
C12 H14 N2 O S
Chemical Catalog
Supplier: ACB Blocks Ltd
STN Files: CHEMCATS

L5 RN ED CN FS MF SR

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

LS ANSWER 221 OF 221 REGISTRY COPYRIGHT 2006 ACS on STN
RN 117866-29-2 REGISTRY
ED Entered STN: 09 Dec 1988
CN Thiazole, 4-(p-methoxyphenyl)-2-{methylaminomethyl}-, hydrochloride (6CI)
(CA INDEX NAME)
MF C12 H14 N2 O S . Cl H
SR CAOLD
LC STN Files: BEILSTEIN*, CAOLD

(*File contains numerically searchable property data)
CRN (100134-70-1)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> fil caold COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 189.68 189.89

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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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=> s 117866-29-2/rn

L6

1 117866-29-2

0 117866-29-2D

1 117866-29-2/RN

(117866-29-2 (NOTI) 117866-29-2D)

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Numbers (AN) CA References.

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PAGE ---- Page Image of original Chemical Abstracts issue containing the abstract of the answer.

PAGE.PREV and PAGE.NEXT will return the image of the page before or after the current answer.

ENTER DISPLAY FORMAT (ALL):all

L6 ANSWER 1 OF 1 CAOLD COPYRIGHT 2006 ACS on STN
AN CA55:25917g CAOLD COMPAGE.
TI complex-forming compds. of the thiazole series
Braun, R. A.; Kuehne, H.; Prijs, B.
IT 18138-21-1 18907-76-1 98428-85-4 99171-57-0 99180-27-5 99853-12-0
100134-70-1 101424-71-9 102309-32-0 102441-11-2 102441-30-5 102956-10-5
102956-41-2 103151-72-0 103155-61-9 103280-39-3 103642-51-9 103642-52-0
104297-14-5 104339-29-9 106652-81-7 109402-49-5 110665-13-9 111209-89-1
112070-95-8 114186-51-5 114278-22-7 114400-20-3 115188-62-0
117866-29-2 120639-50-1 120639-52-3

=> d bib hitstr

ANSWER 1 OF 1 CAOLD COPYRIGHT 2006 ACS on STN CA55:25917g CAOLD complex-forming compds. of the thiazole series Braun, H. A., Kuehne, H.; Prijs, B. 117866-29-2 117866-29-2 CAOLD Thiazole, 4-(p-methoxyphenyl)-2-(methylaminomethyl)-, hydrochloride (6CI) (CA INDEX NAME)

• HC1

=> fil reg
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 8.64 198.53

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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http://www.cas.org/ONLINE/UG/regprops.html

=> fil caplus COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.44 198.97

FULL ESTIMATED COST

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=> d his

(FILE 'HOME' ENTERED AT 08:44:35 ON 24 MAY 2006)

FILE 'REGISTRY' ENTERED AT 08:44:42 ON 24 MAY 2006

L1 STRUCTURE UPLOADED

L2 12 S L1

L3 336 S L1 FULL

L4 115 S L3 AND CAPLUS/LC

L5 221 S L3 NOT L4

FILE 'CAOLD' ENTERED AT 08:46:33 ON 24 MAY 2006 L6 1 S 117866-29-2/RN

FILE 'REGISTRY' ENTERED AT 08:48:10 ON 24 MAY 2006

FILE 'CAPLUS' ENTERED AT 08:48:13 ON 24 MAY 2006

=> s 14

L7 18 L4

=> d ibib abs hitstr 1-18

L7 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2006 ACS ON STN ACCESSION NUMBER: 2006:117229 CAPLUS DOCUMENT NUMBER: 144:212766

DOCUMENT NUMBER:

144:212766
Preparation of thiazolyl-containing benzamidines for prevention and treatment of osteoporosis, bone fractures and allergic inflammatory diseases Lee, Jin Soo: Ahn, Seok Hoon; Jin, Young Goo: Jin, Sang Mi: Park, Whui-Jung; Ku, Sae Kwang; Hwang, Yun Ha; Kim, Pan Soo; Yi, Sun Shin; Ryu, Jei Man Dong Whe Pharmaceutical. Ind. Co., Ltd., S. Korea PCT Int. Appl., 186 pp.
CODEN: PIXXD2 INVENTOR(S):

PATENT ASSIGNEE (S):

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA	TENT	NO.			KIN	D	DATE			APPL	ICAT		DATE					
						-									-			
WO	2006	50140	87		A1		2006	0209	1	WO 2	005-	KR25	45		20050804			
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		CN,	co,	CR.	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KM,	KP,	KZ,	LC,	
		LK,	LR.	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NG,	
		NI.	NO.	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	
		SM,	SY,	TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	
		ZM,	ZW															
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		CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,	
		GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,	
					D		-											

A 20040804

KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.: KR 2004-61481

OTHER SOURCE(S):

MARPAT 144:212766

AB The present invention relates to thiazolyl-containing benzamidines (shown as

ANSWER 1 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

(drug candidate; prepn. of thiazolyl-contg. benzamidines for prevention

and treatment of osteoporosis, bone fractures and allergic

inflammatory

mmmatory
diseases)
875486-62-7 CAPLUS
Benzenecarboximidamide, 4-{[5-[4-[2-(aminomethyl)-5-(phenylmethyl)-4thiazolyl]phenoxy[pentyl]oxy]-N-hydroxy- (9CI) (CA INDEX NAME)

875486-64-9 CAPLUS

Benzenecarboximidamide, 4-[[5-[4-[2-(aminomethyl)-5-(1-methylethyl)-4-thiazolyl]phenoxy]pentyl]oxy]-N-hydroxy- (9CI) (CA INDEX NAME)

875486-73-0 CAPLUS

Benzenecarboximidamide, 4-[[5-[4-[2-(aminomethyl)-5-ethyl-4-thiazolyl]phenoxy]pentyl]oxy]-N-hydroxy- (9CI) (CA INDEX NAME)

3

REFERENCE COUNT:

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 1 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
I; variables defined below; e.g. N-hydroxy-4-[5-[4-(5-methyl-2-isopropyl-1,3-thiazol-4-yl)phenoxy]pentoxy]benzamidine (shown as II)), a process

the preps. thereof and pharmaceutical comps. comprising the same. The novel benramidine derivs. of the present invention are useful for the prevention and treatment of osteoporosis, bone fractures and allergic inflammatory diseases. For I: R1 is C1-C6 alkyl, C3-C5 cycloalkyl, Ph, benzyl, pyridinyl, guanidino, NNSGR7, CHZNNGR7, M(CHZCH2)2Y, A-N(CH2)n is C1-C6 alkyl which is substituted by pyridine or N(CHZCH2)2Y wherein N(CHZCH2)2Y is (un)substituted by hydroxy, pyridinyl or N(CHZCH2)2Y which is substituted by C1-C6alkyl, R2 is H, C1-C6 alkyl, C3-C6 cycloalkyl, Ph, benzyl, C1-C6 alkyl, which is substituted by hydroxy, C1-C6 alkoxy, halogen or C3-C6 cycloalkyl, C2-C6alkenyl. R3 and R4, each independently, = H, halogen, hydroxy, 6

alkyl which is (un)substituted by halogen, C3-C6 cycloalkylamino, C1-C6 alkoxy, C1-C6 alkanoyloxy, C2-C6 alkenyloxy, phenyl-C1-C6 alkoxy,

alkoxy, C1-C6 alkanoyloxy, C2-Co alkenyloxy, phenoxy,
C2-C6 alkenoyloxy or phenyl-C1-C6 alkanoyloxy, C3-C6 cycloalkyloxy which
is substituted by carboxy, esterified carboxy or aminoxy; R5 is H or hydroxy; Y is O, S, NR6, or CH2; X1 and X3, each
independently, = O, S, NH, N-C1-C6 alkyl, N-C3-C6 cycloalkyl, N-benzyl,
N-phenyl; X2 is C3-C7 alkylene, C1-C3 alkylene-alkenylene-C1-C3-alkylene,
C1-C3 alkylene-C1-C3 alkylene, C1-C3 alkylene-S-C1-C3 alkylene, C1-C3
alkylene-NH-C1-C3 alkylene, C1-C3 alkylene-phene-C1-C3 alkylene,
C1-C3 alkylene, C1-C3 alkylene, C1-C3 alkylene, C1-C3 alkylene,
C3-C7 alkylene which is substituted by C1-C3 alkyl and hydroxy,
C3-C7 alkylene c3-C7 alkylene which is interrupted by
piperazine;

alkylene, C3-C7 alkylene which is substituted by C1-C3 alkyl and nygroxy, C3-C7 alkylene, C3-C7 alkylene which is substituted by C3-C7 alkylene-carbonyl, C3-C7 alkylene which is interrupted by piperazine;
addnl. details including provisos are given in the claims. Percent inhibitory activity of 2000 examples of I on osteoclastogenesis, bone-forming activity of 10 examples of I, on osteoclastogenesis, bone-forming activity of 10 examples of I, inhibition of decrease of bone vol. induced by ovariectomy in mice by 20 examples of I, decrease of a substance-dosing groups compared to that of the vehicle control in a rib fracture-induced rat model by 5 examples of I, decrease of abs. and relative lung wts. compared to that of the vehicle control in a mouse model of asthma induced with ovalbumin by 7 examples of I, decrease of total leukocytes in peripheral blood and BALF compared to that of the vehicle control in an asthmatic model, cytotoxicity towards MC3T3-E1 and ST2 cells by 44 examples of I are tabulated. Methods of prepn. are claimed and prepns. and/or characterization data for >200 examples of I hydroxylamine

hydroxlamine

hydroxlamine

hydroxlorioride to 4-{5-(4-(5-methyl-2-isopropyl-1, 3-thiazol-4-yl)phenoxylpentoxylbenzonitrile, which was prepd. in 6 steps (90.3, 98, 70, 80, 95, 89 %) starting from 4-hydroxyhenzonitrile and 1-bromo-5-chloropentane and involving intermediates 4-{5-(4-(propionylphenyl)porphenazylopenzonitrile, and 4-[5-(4-(2-bromopropionyl)phenoxylpentoxylbenzonitrile, and 4-[5-(4-(2-bromopropionyl)phenoxylpenzonitrile.

17 875486-62-7P, N-Hydroxy-4-{5-(4-(2-aminomethyl-1-)a-benzyl-1,3-thiazol-4-yl)phenoxylpentoxylbenzamidine 875486-73-0P, N-Hydroxy-4-{5-(4-(2-aminomethyl-1,3-thiazol-4-yl)phenoxylpentoxylbenzamidine 875486-73-0P, N-Hydroxy-4-{5-(4-(5-ethyl-2-aminomethyl-1,3-thiazol-4-yl)phenoxylpentoxylbenzamidine 875486-73-0P, N-Hydroxy-4-{5-(4-(5-ethyl-2-aminomethyl-1,3-thiazol-4-yl)phenoxylpentoxylbenzamidine 875486-73-0P, N-Hydroxy-4-(5-(4-(5-ethyl-2-2-aminomethyl-1,3-thiazol-4-yl)phenoxyl

L7 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS ON STN ACCESSION NUMBER: 2005:140811 CAPLUS DOCUMENT NUMBER: 142:240429
TITLE: Five-membared

142:240429
Five-membered heterocycle derivatives useful as monoamine oxidase inhibitors, lipid peroxidation inhibitors, and sodium channel modulators, and the production thereof, and use thereof as medicaments Chabrier De Lassauniere, Pierre-etienne: Harnett, Jermiah; Bigg, Dennis; Liberatore, Ann-Marie; INVENTOR (S): Pommier,

Jacques: Lannoy, Jacques: Thurieau, Christophe: Dong,

PATENT ASSIGNEE(S):

Fr. U.S. Pat. Appl. Publ., 154 pp., Cont.-in-part of U.S. Ser. 601,002. CODEN: USXXCO

DOCUMENT TYPE: Patent English

FAMILY ACC. NUM. COUNT:

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-	P	:	AT.	BE.	CH.	DE.	DK.	ES,	FR.	GB.	GR.	IT.	LI.	LU.	NL.	SE.	MC,	PT,
			TE.	ST.	LT.	T.V.	FT.	CY										
F	R 28	23	208	,		Ai		2002	1011		FR 2	001-	4943			21	00104	410
F	R 28	23	208			Bl		2004	0319									
W	0 20	02	0836	56		A2		2002	1024		NO 2	002-	FR12	18		21	00204	409
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	W	:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
			co,	CR,	cu,	cz,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GΕ,	GH,
			GΜ,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KΡ,	KR,	ΚZ,	LC,	LK,	LR,
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	NZ,	OM,	PH,
								SE,				SL,	TJ,	TM,	TN,	TR,	TT,	TZ,
			UA,	UG,	US,	UZ,	VN,	YU,	ZΑ,	ZM,	ZW							
	R	W:	GH,	GΜ,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	υG,	ZM,	ZW,	ΑT,	BE,	CH,
			CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,
			BF,	BJ,	CF,	CG,	CI,	CH,	GΑ,	GN,	GQ,	G₩,	ML,	MR,	ΝE,	SN,	TD,	TG
Z.	A 20	03	0077	50		А		2004	0726		ZA 2	003-	7750			21	30310	003
U	S 20	04	1327	88		A1		2004	0708		US 2	003-	6810	0Z		21	30310	008
W	0 20	05	0355	10		A1		2004 2004 2005	0421		WO 2	004-	FR25	31		21	30410	008

CAPLUS COPYRIGHT 2006 ACS ON STN AL, AM, AT, AU, AZ, BA, BB, BG, BR, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, GH, RH, HU, ID, IL, IN, IS, JP, KE, LS, LT, LU, LV, MA, MD, MG, MK, MM, OM, FG, FH, FL, FT, RO, RU, SC, SD, TH, TR, TT, TZ, UA, UG, US, UZ, VC, GK, KE, LD, RW, MZ, NA, SD, SL, SZ, FI, FR, GB, GR, HU, IE, IT, LU, MC, IT, RB, BB, GC, CI, CM, GA, GN, GT, CG ANSWER 2 OF 18
W: AE, AG,
CN, CO,
GE, GH,
LK, LK,
NO, NZ,
TJ, TM,
RW: BW, GH,
AZ, BY,
EE, ES,
SI, SK,
SN, TD,
ORLTY APPLN, INFO L7 (Cont BW, BY, EG, ES, KG, KP, MW, MX, SE, SG, VN, YU, TZ, UG, CH, CY, BZ, FI, KR, MZ, SK, ZA, ZM, CZ, PT, ML, NL, GQ, PRIORITY APPLN. INFO. : FR 1999-12643 A 19991011 FR 2000-10151 A 20000801 FR 2000-11169 A 20000901 WO 2000-FR2B05 W 20001010 FR 2001-4943 A 20010410 FR 2002-1811 A 20020214 US 2002-89993 A2 20020404 WO 2002-FR1218 A1 20020409 US 2003-681002 A2 20031008 A3 20001010 EP 2000-967988 US 2004-915001 A 20040810 OTHER SOURCE(S): MARPAT 142:240429

ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continus sodium channels in rat cerebral cortex homogenates. 218946-61-7P, 4-{3,5-Bis(1,1-dimethyle-thyl)-4-hydroxyphenyl|-N-methyl-2-thiazolemethanamine 335242-74-5P, Benzyl L7 (Continued)

[{4-[3,5-di(tert-butyl)-4-hydroxyphenyl]-1,3-thiazol-2-yl]methyl]carbamate 335242-75-6P, 4-[2-(Aminomethyl)-1,3-thiazol-4-yl]-2,6-di(tert-butyl)phenol 335242-76-7P, 2,6-Di(tert-butyl)-4-[2-[[(methyl)(4-nitrobenzyl)amino]methyl]-1,3-thiazol-4-yl]phenol 335242-78-9P, 2,6-Di(tert-butyl)-4-(2-[[(4-nitrobenzyl)amino]methyl]-1,3-thiazol-4-yllphenol

inhibitors, lipid peroxidm. inhibitors, and sodium channel modulators) 218944-61-7 CAPLUS MAO

CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-{2-{(methylamino)methyl}-4-thiazolyl}-(9CI) (CA INDEX NAME)

335242-74-5 CAPLUS Carbmic acid, [14-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

335242-75-6 CAPLUS
Phenol, 4-[2-(aminomethyl)-4-thiezolyl)-2,6-bis(1,1-dimethylethyl)- (9CI)
(CA INDEX NAME)

335242-76-7 CAPLUS RN

ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN

The invention relates to pharmaceutical use of heterocyclic compds. of general formula Het(A) (B) - (CH2)n-CR1R2-Q [I; wherein the substituted heterocyclic ring Het(A) (B) = Q1-Q4; A = various aryl or heteroaryl systems, especially a substituted Ph or biphenyl radical, or also alkyl, cycloalkyl, or cycloalkylalkyl; B = especially H or alkyl, or also aryl

substituted alkyl; X = especially NH or S, or also substituted NH; Y = O or S; n = 0-6; R1, R2 = especially H, alkyl, or cycloalkyl; Q = NR3R4 or OR5; R3

**
= especially H, alkyl, cycloalkyl, alkynyl, cyanoalkyl alkoxycarbonyl, aralkoxycarbonyl or (cycloalkyl)oxycarbonyl; R5 = H, alkyl, alkynyl, cyanoalkyl]. I and their racemates, enantiomers, and/or salts can be

for producing medicaments for inhibiting monoamine oxidases (MAO), inhibiting lipid peroxidn., and/or for acting as modulators of sodium channels. The resulting medicaments are particularly for use in treating neurodegenerative disorders such as Parkinson's disease, Alzheimer's disease, Huntington's chorea, amyotrophic lateral sclerosis, or pain. Approx. 500 synthetic examples of I and their salts are given, and numerous free bases of I are claimed. For instance, protection of sarcosinamide-HCl with BOC anhydride gave 72% BOC-N(Me)CH2CONH2, which

converted to the thioamide with (P2S5)2 in 65% yield. Cyclocondensation of the thioamide with 2-bromo-1-(3,5-di-tert-butyl-4-hydroxyphenyl)ethanome (28%), followed by deprotection (73%) and salification (92%), gave thiazole derivative II as the HCl salt. II

salification (97%), gave chaeses described inhibited of the NAO-B specific ligand [3H]-Ro-19-6327 to rat mitochondrial prepns. with IC50 < 10 wM. Selected I also inhibited formation of malondialdehyde by lipid peroxidn. in rat cerebral cortex prepns., and inhibited specific binding of [3H]-batrachotoxin to voltage-dependent

ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[[methyl](4-nitrophenyl)methyl]amino]methyl]-4-thiazolyl}- (9CI) (Continued) (CA INDEX NAME)

$$\begin{array}{c} \text{t-Bu} \\ \text{ho} \\ \text{t-Bu} \end{array}$$

335242-78-9 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[[[(4nitrophenyl)methyl]amino]methyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

335242-67-6P, 2,6-Di(tert-butyl)-4-{2-[[methyl(2-propynyl) amino]methyl]-1,3-thiazol-4-yl]phenol 335242-68-7P, 2-[[(4-[3,-bl) (tert-butyl)-4-hydroxyphenyl)-1,3-thiazol-2-yl]methyl [methyl] amino]acetonitrile 335242-69-8P, 5-[[(4-[3,-bl) (tert-butyl)-4-hydroxyphenyl)-1,3-thiazol-2-yl]methyl [methyl] amino]pentamenitrile 335242-70-1P, 6-[[(4-[3,-bl) (tert-butyl)-4-hydroxyphenyl)-1,3-thiazol-2-yl]methyl [methyl] amino]pentamenitrile 335242-70-1P, 6-[[(4-[3,-bl) (tert-butyl)-4-[2-[([2-hydroxyethyl) (methyl) amino]methyl]-1,3-thiazol-4-yl]phenol 335242-72-3P, 4-[2-[[(4-Aminobenzyl) (methyl) amino]methyl]-1,3-thiazol-4-yl]-2,6-di(tert-butyl)-phenol 335242-77-8P, 4-[2-[[(4-Aminobenzyl) amino]methyl]-1,3-thiazol-4-yl]-2,6-di(tert-butyl)-phenol 335242-79-9P, 4-[2-[[(4-Aminobenzyl) amino]methyl]-1,3-thiazol-4-yl]-2,6-di(tert-butyl)-phenol 335242-79-3P, (2-6-Di-tert-butyl)-4-([2-[[(4-Aminobenzyl) amino]methyl]-1,3-thiazol-4-yl]-2,6-di(tert-butyl)-4-([2-[[(4-Aminobenzyl) amino]methyl]-1,3-thiazol-4-yl]-1,0-thiazol-2-P, 2,6-Di-tert-butyl-4-([2-([(4-Aminobenzyl) amino]methyl]-1,3-thiazol-4-yl]phenol 335246-31-0P, 4-[2-[((4-Aminobenzyl) amino]methyl]-1,3-thiazol-4-yl]phenol hydrochloride 335246-31-0P, 4-[2-([(4-Aminobenzyl) amino]methyl]-1,3-thiazol-4-yl]phenol hydrochloride 335246-31-0P, 4-[2-([(4-Minobenzyl) amino]methyl]-1,3-thiazol-4-yl]phenol hydrochloride 335246-31-0P, 4-[2-([(4-Minobenzyl) amino]methyl]-1,3-thiazol-4-yl]phenol 335246-31-0

(drug candidate; preparation of five-membered heterocycle derivs. as

MAC

L7 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) inhibitors, lipid peroxidn. inhibitors, and sodium channel modulators)
RN 335242-67-6 CAPLUS
Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[(methyl-2-propynylamino)methyl]-4-thiszolyl]- (GCI NDEX NAME)

335242-68-7 CAPLUS
Acetonitrile, [[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]methylamino]- [9CI] (CA INDEX NAME)

335242-69-8 CAPLUS Pentanenitrile, 5-[[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methylmethylaminoj- (9CI) (CA INDEX NAME)

335242-70-1 CAPLUS

Hexanenitrile, 6-[[[4-[3,5-bis(1,1-dimethylethyl])-4-hydroxyphenyl]-2-thiazolyl]methyl]methylamino]- (9CI) (CA INDEX NAME)

RN 335242-71-2 CAPLUS CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[[(2-hydroxyethyl)methylamino]methylethyl)-4-[2-[[(2-hydroxyethyl)methylamino]methylethyl)methylamino]methylamino]methylethylamino]methylamino[methylamino]methylamino[methylamino]methylamino[methylamino]methylamino[methylamino]methylamino[methylamino]methylamino[methylamino]methylamino[methylamino]methylamino[methylamino]methylamino[methylamino]methylamino[methylamino]methylamino[methylamino]methylamino[methylamino]methylamino[methylamino]methylamino[methylamino[methylamino]methylamino[methylamino[methylamino[methylamino[methylamino]methylamino[methyl 335242-71-2 CAPLUS

ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

335242-82-5 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[[[(3-nitrophenyl)methyl]amino]methyl]-4-thiazolyl](CA INDEX NAME)

335245-99-3 CAPLUS
Phenol, 4-[2-[methylamino)methyl]-4-thiazolyl]-2,6-bis[1-methylethyl]-,
hydrochloride [9CI] (CA INDEX NAME)

335246-01-0 CAPLUS
Phenol, 4-[2-[(methylamino)methyl]-4-thiazolyl]-, hydrochloride (9CI) INDEX NAME)

ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN y1]-4-thiazoly1]- (9CI) (CA INDEX NAME) (Continued)

RN 335242-72-3 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[[methyl(phenylmethyl)amino]methyl
]-4-thiazolyl]- (9CI) (CA INDEX NAME)

$$\Pr_{\mathsf{Ph-CH}_2-\mathsf{N-CH}_2} \stackrel{\mathsf{t-Bu}}{\underset{\mathsf{S}^{\mathsf{u}}}{\longrightarrow}} \mathsf{OH}$$

335242-77-8 CAPLUS

PRENDI, -{[[[(4-minophenyl)methyl]methylamino]methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl}- (9CI) (CA INDEX NAME)

335242-79-0 CAPLUS
Phenol, 4-[2-[[[(4-aminophenyl)methyl]amino]methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

335242-81-4 CAPLUS
Butanenitrile, 4-{[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methylmethylamino]- (9CI) (CA INDEX NAME)

ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continue 335246-05-4 CAPLUS Phenol, 4-[2-[(dimethylamino)methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)-, hydrochloride (9CI) (CA INDEX NAME) (Continued)

$$\begin{array}{c} \text{t-Bu} \\ \text{OH} \\ \text{Me}_2\text{N-CH}_2 \\ \text{s} \end{array} \begin{array}{c} \text{OH} \\ \text{Bu-t} \end{array}$$

●x HCl

335246-19-0 CAPLUS

335246-31-6 CAPLUS
Phenol, 4-{2-{(methylamino)methyl]-4-thiazolyl}-2,6-bis(1-methylethyl)-(9C1) (CA INDEX NAME)

335246-32-7 CAPLUS
Phenol, 4-[2-[(methylamino)methyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

335246-34-9 CAPLUS
Phenol, 4-[2-[(dimethylamino)methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

218944-60-6F, 4-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-N[(1,1-dimethylethoxy)carbonyl]-N-methyl-2-thiazolemethanamine
335247-51-3F, 4-[2-[[(tert-Butoxycarbonyl](methyl)amino]methyl]1,3-thiazol-4-yl]-2,6-diisopropylphenyl acetate 335247-52-6F,
tert-Butyl [[4-(4-hydroxy-3,5-diisopropylphenyl]-1,3-thiazol-2yl]methyl](methyl]carbamate acetate 335247-53-5F, tert-Butyl
[[4-(4-hydroxyphenyl)-1,3-thiazol-2-yl]methyl](methyl]carbamate
RL: RCT (Reactant) SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(intermediate: preparation of five-membered heterocycle deriva. as RAO
inhibitors, lipid peroxidn. inhibitors, and sodium channel modulators)
218944-60-6 CAPLUS
Carbamic acid, [[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2thiazolyl]methyl;methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

335247-51-3 CAPLUS
Carbamic acid, [[4-[4-[acetyloxy]-3,5-bis[1-methylethyl]phenyl]-2thiazolyl]methylmethylmethyl-, 1,1-dimethylethyl ester (9C1) (CA INDEX NAME)

ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

● HC1

717915-30-5 CAPLUS Glycine, N-[(4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyll-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

473540-20-4P 473540-21-5P 473540-24-0P 473540-22-PP 473540-28-2P 473540-29-3P 473540-30-8P 473540-39-4P 473540-38-4P 473540-38-4P 473540-38-4P 473540-38-4P 473540-38-4P 473540-38-4P 473541-30-3P 473541-36-3P 47354

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of five-membered heterocycle derivs. as MAO inhibitors,

lipid

peroxidn. inhibitors, and sodium channel modulators)
473540-20-4 CAPLUS
Phenol. 2, 6-bis(1,1-dimethylethyl)-4-[2-[2-(methylamino)ethyl]-4thiazolyl]-, monohydrochloride (9CI) (CA INDEX NAME)

L7 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN

335247-52-4 CAPLUS
Carbamic acid, [[4-[4-hydroxy-3,5-bis(1-methylethyl)phenyl]-2-thiazolyl]methyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

335247-53-5 CAPLUS Carbamic acid, [[4-(4-hydroxyphenyl)-2-thiazolyl]methyl]methyl-, 1,1-dimethylethyl ester [9CI] (CA INDEX NAME)

473541-41-2P 717915-30-5P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); TRU (Therapeutic use); BlOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of five-membered heterocycle derivs. as MAO inhibitors,

peroxidn. inhibitors, and sodium channel modulators)
RN 473541-41-2 CAPLUS
CN Phenol,
2,6-bis[1,1-dimethylethyl]-4-[2-{{methylamino}methyl}-4-thiazolyl}, monohydrochloride (9CI) (CA INDEX NAME)

L7 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

● HCl

473540-21-5 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[1-(methylamino)ethyl]-4-thiazolyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

473540-24-8 CAPLUS Acctande, N-[4+-3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]- (9CI) (CA INDEX NAME)

473540-25-9 CAPLUS Carbamic acid, ([4-(3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl|methyl]-, ethyl ester (9CI) (CA INDEX NAME)

ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continu 473540-28-2 CAPLUS Phenol, bis(1,1-dimethylethyl)-4-{2-{(phenylamino)methyl}-4-thiazolyl}-(9CI) (CA INDEX NAME)

473540-29-3 CAPLUS
Phenol, 4-[2-[[[2-(dimethylamino)ethyl]methylamino]methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

473540-30-6 CAPLUS
Phenol, 2.6-bis(1,1-dimethylethyl)-4-{5-methyl-2-((methylamino)methyl)-4-thiazolyl|-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

473540-32-8 CAPLUS Acetamide, N-[(14-13,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl)-2-thiazolyljmethyl)-N-methyl- (9CI) (CA INDEX NAME)

ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

● HC1

473540-68-0 CAPLUS

CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[(propylamino)methyl]-4-thiazolyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 473540-86-2 CAPLUS
CN Phenol,
4-[2-[(butylamino)methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl), monohydrochloride (9CI) (CA INDEX NAME)

• HC1

RN 473540-96-4 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-{2-{2-methyl-1-(methylamino)propyl}-4-thiazolyl}-, monohydrochloride (9CI) (CA INDEX NAME)

L7 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 473540-34-0 CAPLUS
CN Phenol,
2,6-bis[1,1-dimethylethyl)-4-[2-[(ethylamino)methyl]-4-thiazolyl], monohydrochloride (9CI) (CA INDEX NAME)

● HC1

473540-38-4 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-([(1-methylethyl)amino]methyl]-4-thiazolyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

473540-39-5 CAPLUS
Phenol, 4-{2-{(cyclohexylamino)methyl]-4-thiazolyl]-2,6-bis(1,1-dimethyl-thyl)-, monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

● HCl

473541-07-0 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[[(phenylmethyl)amino]methyl]-4-thiazolyl]-, monohydrochloride (SCI) (CA INDEX NAME)

● HC1

473541-32-1 CAPLUS
Carbamic acid, [[4-{3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl}-2-thiazolyl}methyl]-, methyl ester (9CI) (CA INDEX NAME)

473541-33-2 CAPLUS
Benzamide, N-[(4-(3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]- (9C1) (CA INDEX NAME)

$$\begin{array}{c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) 473541-34-3 CAPLUS Benzeneacetamide, N-[(4-{3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl}-2-thiazolyl|methyl]- (9CI) (CA INDEX NAME)

473541-35-4 CAPLUS
Propanamide, N-[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiezolyl|methyl]- (9CI) (CA INDEX NAME)

473541-50-3 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[2-(methylamino)ethyl]-4-thiazolyl]-[9CI) (CA INDEX NAME)

473541-51-4 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[1-(methylamino)ethyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

473541-53-6 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[5-methyl-2-[(methylamino)methyl]-4-tiazolyl]- (9CI) (CA INDEX NAME)

ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 473541-80-9 CAPLUS
CN Phenol,
4-[2-[(butylamino)methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)(9C1) (CA INDEX NAME)

RN 473541-82-1 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[2-methyl-1-(methylamino)propyl]-4thiarolyl]- (9CI) (CA INDEX NAME)

473541-85-4 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[[(phenylmethyl)amino]methyl]-4-thiazolyl]- (SCI) (CA INDEX NAME)

RN 717915-11-2 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[3-methyl-1-(methylamino)butyl]-4thiazolyl]-, monohydrochloride (9CI) (CA INDEX NAMZ)

L7 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

473541-56-9 CAPLUS

RN 473541-56-9 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[(ethylamino)methyl]-4-thiazolyl]{9CI} (CA INDEX NAME)

473541-60-5 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-{2-[{(1-methylethyl)amino]methyl}-4-thiazolyl]- (9CI) (CA INDEX NAME)

473541-61-6 CAPLUS
Phenol, 4-[2-[(cyclohexylamino)methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

473541-69-4 CAPLUS

RN 473541-69-4 CAPLUS
CN Phenol,
2,6-bis[1,1-dimethylethyl]-4-[2-[(propylamino)methyl]-4-thiazolyl](9CI) (CA INDEX NAME)

L7 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

717915-19-0 CAPLUS Phenol, 2.6-bis(1,1-dimethylethyl)-4-[2-[(1S)-1-(methylamino)ethyl]-4-thiazolyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

717915-23-6 CAPLUS Phenol, 2,6-bis(1,1-dimethylethyl)-4-{2-[(1R)-1-(methylamino)ethyl]-4-thiszolyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

717915-32-7 CAPLUS Glycine, N-[[4-{3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl)-2-thiazoly]|methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

717915-36-1 CAPLUS
Glycine, N-[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2thiazolyl]methyl]- (9CI) (CA INDEX NAME)

RN 717915-49-6 CAPLUS
CN Phenol,
4-[2-[(IR)-1-aminoethyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)-,
monohydrochloride (9CI) (CR INDEX NAME)

Absolute stereochemistry.

• HC1

717915-51-0 CAPLUS

CN Phenol, 4-{2-{(1S)-1-aminoethyl}-4-thiazolyl}-2,6-bis(1,1-dimethylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

717915-79-2 CAPLUS Glycine, N-[(4-(3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

717915-85-0 CAPLUS Phenol, 4-[2-[(1R)-1-aminoethyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)-(9C1) (CA INDEX NAME)

Absolute stereochemistry.

717915-86-1 CAPLUS
Phenol, 4-[2-[(1S)-1-aminoethyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

● HC1

717915-62-3 CAPLUS
Glycine, N-[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2thiazolyl]mathyl]-N-(2-ethoxy-2-oxoethyl)-, ethyl ester,
hydroxblogide hydrochloride (9CI) (CA INDEX NAME)

• HC1

RN 717915-74-7 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[3-methyl-1-(methylamino)butyl]-4thiazolyl]- (9CI) (CA INDEX NAME)

717915-77-0 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[(1S)-1-(methylamino)ethyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 2 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) 845643-59-6 CAPLUS Acctamide, 2-{[[4-{3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} & & & \\ & &$$

● HC1

473541-38-79 717915-34-99 845643-61-09
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of five-membered heterocycle derivs. as MAO inhibitors, IT

lipid

peroxidn. inhibitors, and sodium channel modulators)
473541-38-7 CAPLUS
Carbamic acid, [2-[4-[3,5-bis[1,1-dimethylethyl]-4-hydroxyphenyl]-2thiazolyl]ethyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

717915-34-9 CAPLUS
Glycine, N-[(4-(3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2thiazolyl]methyl]-M-[(1,1-dimethylethoxy)carbonyl]- (9CI) (CA INDEX

845643-61-0 CAPLUS Glycine, N-[(4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl)-2-thiazolyl]methyl]-N-[(1,1-dimethylethoxy)carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

ANSWER 3 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

AB Title compds. I [V = N, CH; W = S, O; m = 0-2; R1, R2 = H, alkyl; X = NR4, etc.; R4 = H, alkyl; n = 0-4; p = 0, 1; L = CR20R21, etc.; R20 = H,

alkyl

aikyi, etc.; R21 = H, alkyi, etc.; R = CO2R19, etc.; R19 = H, alkyi; B = aryi, heteroaryi; R3 = H, halo, etc.; Y = O, etc.; s = O, 1; A = (un)substituted substituted alkylene with cycloalkyl; Z = cycloalkyl, etc.} were prepared For

example pre, O-alkylation of 5-hydroxynicotinic acid Me ester with compound II [Q =

C1], e.g., prepared from 4-bromoacetylbenzoic acid in 5 steps, followed by saponification

afforded compound II [3-carboxypyridin-5-yloxy] in 44.1% overall yield. PTP1B (protein tyrosine phosphatase 1B) inhibition assays, the IC50 value of compound II $\{Q=3\text{-}carboxypyridin-5-yloxy}\}$ was 0.28 μM . Compds. I

are claimed useful for the treatment of obesity, diabetes, etc. Formulations

claimed useful for the treatment of our given.
776309-65-09 776309-66-19 776309-69-49
776309-70-79 776309-71-89 776309-72-99
776309-73-09 776309-74-19 776309-75-29
776310-81-779 776310-82-89 776310-86-29
776310-81-79 776310-88-49 776310-89-59
11. DEC [Obs. mosclotical activity). SI

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (USes) (preparation of azole compds. as PTP1B inhibitors for treatment of

obesity

and diabetes) 776309-65-0 CAPLUS

L7 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2006 ACS ON STN ACCESSION NUMBER: 2004:878382 CAPLUS DOCUMENT NUMBER: 141:350161 Preparation of azole compounds

141:350161
Preparation of azole compounds as PTPlB inhibitors
Ikemoto, Tomoyuki; Tanaka, Masahiro: Yuno, Takeo;
Sakamoto, Johei: Nakanishi, Hiroyuki; Nakagawa,
Yuichi: Ohta, Takeshi; Sakata, Shohei: Morinaga,
Hisayo
Japan Tobacco Inc., Japan
PCT Int. Appl., 542 pp.
CODEN: PIXXD2
Patent
Japanese
1 INVENTOR (S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT:

	PA'	TENT	NO.			KIN	D	DATE			APPI	ICAT	ION	NO.		Đ	ATE		
	WO	2004	0899	18		A1		2004	1021		WO 2	004-	JP51	19		2	0040	409	
												BG,							
												EC.							
			GE,	GH,	GM.	HR.	HU.	ID.	IL.	IN.	IS.	JP,	KE,	KG,	KP,	KR,	KZ,	LC.	
			LK,	LR,	LS,	LT.	LU,	LV.	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,	
			NO,	NZ,	OM,	PG.	PH,	PL.	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	
			TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW	
		RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	
			BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	cz,	DE,	DK,	EE,	
			ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	
			SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CH,	GΑ,	GN,	GQ,	G₩,	ML,	MR,	ΝE,	SN,	
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HR																			
	BR	2004	0091	36		Α.		2006	0425	1	BR 2	004-	9136			2	0040	409	
	JP	2005	2724	76		A2		2005	1006	•	JP 2	005-	1337	55		2	0050	428	
	NO	2005	0052	46		A		2005	1221		NO Z	005-	5246			. 2	0051	108	
PRIO	JP 2005272476 NO 2005005246 DRITY APPLN. INFO.:				. :						JP 2	003-	1052	67		A Z	0030	409	
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											JP Z	003-	13/3	90		A 2	0030	603	
											TD 2	005-					0040	400	
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											2	004-	, . J L	• •			0040	-03	

OTHER SOURCE(S):

L7 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN CN Glycine, (Continued)

MARPAT 141:350161

GIYGINe, henylmethyl)-N-[[4-[4-[(4-[1-propylbutyl)phenyl]methoxy]pheny l]-2-thiazolyl]methyl]- (9CI) (CA INDEX NAME)

776309-66-1 CAPLUS Glycine, N-[(4-[4-[4-(1-ethylpropyl)phenyl]methoxy]phenyl]-2-thiazolyl]methyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Ph-CH2} \\ \text{HO}_2\text{C-CH}_2 - \text{N-CH2} \\ \end{array} \\ \begin{array}{c} \text{N} \\ \text{CHEt2} \end{array}$$

776309-69-4 CAPLUS
Glycine, N-[[4-[4-[4-(1-ethylpropyl)phenyl]methoxy]phenyl]-2thiazolyl]methyl]-N-[(4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)

776309-70-7 CAPLUS
Glycine, N-[[4-[4-[4-(1-ethylpropyl)phenyl]methoxy]phenyl]-2thiazolyl]methyl]-N-[[4-(1-methylethyl)phenyl]methyl]- (9CI) (CA INDEX
NAME)

776309-71-8 CAPLUS
Glycine, N-{[4-{4-(1-ethylpropyl)phenyl]methoxy]phenyl]-2thiazolyl]methyl]-N-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX
NAME)

ANSWER 3 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

776309-72-9 CAPLUS
Glycine, N-[(4-chlorophenyl)methyl]-N-[(4-[4-[4-(1-ctyl/popyl)phenyl)methoxy]phenyl]-2-thiazolyl)methyl]- (9CI) (CA INDEX

776309-73-0 CAPLUS
Glycine, N-[(3,5-dimethylphenyl)methyl]-N-[[4-[4-[1-ethylpropyl)phenyl]methoxylphenyl]-2-thiazolyl[methyl]- (9CI) (CA INDEX NAME)

776309-74-1 CAPLUS Glycine, N-[[4-(4-([4-(1-propylbutyl)phenyl]methoxy]phenyl]-2-thiazolyl]methyl]-N-(2-pyridinylmethyl)- (SCI) (CA INDEX NAME)

776309-75-2 CAPLUS Glycine, N-[{4-{4-[1-ethylpropyl)phenyl}methoxy]phenyl}-2-thiazolyl}methyl]-N-{2-pyridinylmethyl}- (9CI) (CA INDEX NAME)

ANSWER 3 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 776310-82-8 CAPLUS

CN Glycine,
N-[2-[[4-(1-methylethyl)phenyl]amino]-2-oxoethyl]-N-[[4-[2-methyl4-[4-(1-propylbutyl)phenyl]methoxy]phenyl]-2-thiazolyl]methyl](CA INDEX NAME)

PAGE 1-B

-- CH (Pr-n) 2

776310-86-2 CAPLUS
Glycine, N-[{4-{2-methyl-4-[{4-{1-propylbutyl}phenyl}methoxy]phenyl}-2-thiazolyl]methyl}-N-{4-thiazolylmethyl}- (9CI) (CA INDEX NAME)

776310-87-3 CAPLUS Glycine, N-[$\{4-\{2-methy\}-4-\{\{4-\{1-propylbuty\}\}pheny\}\}methoxy]phenyl\}-2-thiazoly]]methyl}-N-{\{2-methy}-4-thiazoly]methyl}-, monohydrochloride (9CI) (CA INDEX NAME)$

L7 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

776309-77-4 CAPLUS
Glycine, N-benzoyl-N-[{4-(4-[[4-(1-propylbutyl)phenyl]methoxylphenyl]-2-thiazolyl]methyl]- (9CI) (CA INDEX NAME) RN CN

776309-78-5 CAPLUS Glycine, N-[(4-(4-(1-ethylpropyl)phenyl]methoxylphenyl]-2-thiazolyl]methyl]-N-(4-methylbenzoyl)- (9CI) (CA INDEX NAME)

$$\begin{picture}(20,0) \put(0,0){\line(0,0){100}} \put(0,0){\line(0,0){100$$

776309-79-6 CAPLUS
Glycine, N-(4-methoxybenzoyl)-N-[[4-[4-(1-propylbutyl)phenyl]methoxy]phenyl]-2-thlazolyl]methyl]- (9CI) (CA INDEX NAME)

776310-81-7 CAPLUS Glycine, N-[[4-(2-methyl-4-[[4-(1-propylbutyl)phenyl]methoxy]phenyl]-2-thiazolyl]methyl]-N-[2-oxo-2-(phenylamino)ethyl]- [9CI) (CA INDEX NAME)

L7 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

776310-88-4 CAPLUS Glycine, N-[{4-{2-methyl-4-{[4-{1-propylbutyl]phenyl]methoxy]phenyl}-2-thiazolyl]methyl-N-[2-oxo-2-{(phenylmethyl)amino]ethyl}-, monohydrochloride (9CI) (CA INDEX NAME)

PAGE 1-B

-CH (Pr-n) 2

776310-89-5 CAPLUS
Glycine, N-(1H-benzimidazol-2-ylmethyl)-N-[[4-[2-methyl-4-[[4-(1-propylbutyl)phenyl]methoxy]phenyl]-2-thiazolyl]methyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT: THIS

THERE ARE 16 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L7 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2006 ACS ON STN ACCESSION NUMBER: 2004:579270 CAPLUS DOCUMENT NUMBER: 142:32843

DOCUMENT NUMBER:

142:32843 Kinetic characterization of novel NR2B antagonists using fluorescence detection of calcium flux Bednar, Bohumil: Cunningham, Michael E.; Kiss, TITLE: AUTHOR (S):

Cheng, Gong: McCauley, John A.; Liverton, Nigel J.;
Koblan, Kenneth S.
Department of Neurology, Merck Research Laboratories,
West Point, PA, 19454, USA
Journal of Neuroscience Methods (2004), 137(2),
247-255
CODEN: JOMEDT: ISSN: 0165-0270
Elsevier Science B.V.
Journal CORPORATE SOURCE:

SOURCE:

CODEN: JAMEDT; ISSN: 0165-0270

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

B To facilitate the discovery of novel N-methyl-d-aspartate (NMDA) receptor antagonists, we have developed a high-throughput functional assay based

fluorescence detection of free intracellular calcium concns. Mouse fibroblast L(tk-) cells expressing human NRIa/NRZB NMDA receptors were plated in 96-well plates and loaded with florescence calcium indicator fluo-3 AM. NRZB antagonists were added after stimulation of NMDA receptors with 10 µM glutamate and 10 µM glycime. Changes in fluorescence after the addition of the antagonists were fitted by a

exponential equation providing kobs. The concentration dependence of kobs Was
linear for all NR2B antagonists at concns. where kobs<0.2 s-1. The

linear for all NRZB antagonists at Commission and Values of kobs for six structurally distinct NRZB antagonists were in the range of 1.1 to 7.5+105 M-1 s-1. These values were several orders of magnitude slower than that obtained for diffusion limited Mg2+ channel block. The rate consts. koff provided the values of t1/2 for dissociation of NRZB antagonists in the range of 1.8 min for ifenprodil to 240 min for the

alowest novel antagonist. The IC50 values obtained from the end-point fluorescence measurements agree with Kd values calculated from kinetic measurements. All kinetic consts., obtained using our fluorescence method, correlate well with data measured by voltage clamp. 807510-12-4
RL: PAC (Pharmacological activity); PKT (Pharmacokinetica); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (kinetic characterization of novel NR2B antagonists using fluorescence detection of calcium flux) 807610-12-4 CAPLUS Benzenenethanol, 4-hydroxy-α-[(15)-1-[[[4-(4-methoxyphenyl)-2-thiazolyl]methyl]amino]ethyl]-, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN SSION NUMBER: 2004:550745 CAPLUS MENT NUMBER: 141:106475 DOCUMENT NUMBER: TITLE:

141:106475
Preparation of 5-membered heterocycle derivatives for treating neurodegenerative disorders or pain Chabrier De Lassauniere, Pierre-Etienner, Harnett, Jeremiah; Bigg, Dennis; Liberatore, Anne-Marie; Pommler, Jacques; Lannoy, Jacques; Thurieau, Christophe USA INVENTOR (S):

PATENT ASSIGNEE(S):

U.S. V.S. Pat. Appl. Publ., 150 pp., Cont.-in-part of U.S. Ser. No. 89,993.
CODEN: USXXCO

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	ENT					_	DATE				LICAT					ATE	
	2004				A1		2004				2003-					0031	
FR	2799	461			Al		2001	0413		FR	1999-	1264	3		1	9991	011
FR	2799	461			B1		2002	0104									
FR	2812	546			A1		2002	0208		FR	2000-	1015	1		2	0000	801
WO	2001	0266	56		A2		2001	0419		WO	2000-	FR28	05		2	0001	010
WO	2001	0266	56		A3		2002	0418									
	W:	ΑĒ,	AG,	AL,	AM,	AT,	ΑU,	ΑZ,	BA,	BE	, BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
		CR,	cu,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES	, FI,	GB,	GD,	GE,	GH,	GM,	HR,
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ΕP	1228				A3		2004										
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							RO,										
ΕP	1589										2005-					0001	
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					LV,												
	2823				A1					FK	2001-	4943			2	0010	410
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	2003	0077	70		٠.		2004	0726		<u>سم</u>	2003- 2004-	7/30	^1		2	0031	003
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FR 2000-10151

A 20000801

L7 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) THERE ARE 47 CITED REFERENCES AVAILABLE FOR REFERENCE COUNT: 47

FORMAT

RECORD. ALL CITATIONS AVAILABLE IN THE RE

(Continued) A 20000901 L7 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN FR 2000-11169 WO 2000-FR2805 w 20001010 FR 2001-4943 A 20010410 FR 2002-1811 A 20020214 US 2002-89993 A2 20020404 EP 2000-967988 A3 20001010 WO 2002-FR1218 A1 20020409 US 2003-681002 A2 20031008 US 2004-915001 A 20040810

OTHER SOURCE(S): MARPAT 141:106475

The invention relates to thiazole, oxazole, imidazole, isoxazole and isoxazoline derivs. of general formula (I) (wherein Ret = thiazole, oxazole, imidazole, isoxazole or isoxazolo an integer from 0 to A = optionally substituted aromatic radical; B = H, alkyl, Ph; R1, R2 = $\frac{1}{2}$

alkyl, cycloalkyl; Ω = NR46R47 or OR48; R46, R47 = H, alkyl, cycloalkyl, (CH2)k-CO2R51; R51 = alkyl, haloalkyl; R48 = H, alkyl].

These compds. have advantageous pharmacol. properties which allow their use in

medicament intended to inhibit monoamine oxidases (MAO) and/or lipidic peroxidm. and/or to act as modulators of the sodium channels and notably their use in therapeutics for treating (1) central or peripheral nervous system, (2) neurodegenerative disorders selected from Parkinson's disease.

Alzheimer's disease, Huntington's chorea and amyotrophic lateral

sclerosis
or (3) pain selected from the group consisting of postoperative pain,
migraine, neuropathic pain, central pain, chronic inflammatory pain and
pain linked to a cancer. Thus,
2-[[[(1,1-dimethylethoxylcarbonylimethyl]a
mino]ethanethioamide (4.3 g, 2.11 mmol) and
2-bromo-1-(3,5-di-tert-butyl-4hydroxyphenyllethanone (6,9 g, 2,11 mmol) were dissolved in 75 mL benzene
under argon atmospheric and stirred at ambient temperature for 12 h to
que, after

ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) workup and silica get chromatog., 4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-N-([1,1-dimethylethoxy)carbonyl]-N-methyl-2-thiazolemethanamine which was treated with CF3CO2H and triethylsilane in 50 mt. CH2Cl2 to give, after workup, 4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-N-methyl-2-thiazolemethanamine (II). II showed IC50 of lower than 10 µM for inhibiting lipid peroxidn. of the cerebral cortex of rats.

of rats.

335242-74-SP, Benzyl ([4-[3,5-di(tert-butyl)]-4-hydroxyphenyl]-1,3thiazol-2-yl]methyl]carbamate 335242-75-6P, 4-[2-(Aminomethyl)1,3-thiazol-4-yl]-2,6-di(tert-butyl)phenol 335246-19-0P,
4-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-N-methyl-2thiazolemethanamine hydrochloride 473540-29-3P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Greparation); RACT (Reactant or reagent); USES (Uses)
(Intermediate; preparation of 5-membered heterocycle derivs. for

335242-75-6 CAPLUS Phenol, 4-[2-(aminomethyl)-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

335246-19-0 CAPLUS

RN 335246-19-0 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[(methylamino)methyl]-4-thiazolyl], hydrochloride (9CI) (CA INDEX NAME)

ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

335247-51-3 CAPLUS
Carbamic acid, [(4-(4-(acetyloxy)-3,5-bis(1-methylethyl)phenyl)-2thiazolyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

335247-52-4 CAPLUS

Carbamic acid, [[4-[4-hydroxy-3,5-bis(1-methylethyl)phenyl]-2-thiazolyl]methyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

335247-53-5 CAPLUS Carbamic acid, [[4-(4-hydroxyphenyl)-2-thiazolyl]methyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

473541-38-7 CAPLUS Carbamic acid (2-14-(3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]ethyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

●x HCl

473540-29-3 CAPLUS
Phenol, 4-[2-[{[2-(dimethylamino)ethyl]methylamino]methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

RN 473541-69-4 CAPLUS
CN Phenol,
2,6-bis[1,1-dimethylethyl]-4-[2-[(propylamino)methyl]-4-thiazolyl](9CI) (CA INDEX NAME)

treating diseases of central or peripheral nervous system, neurodegenerative

disorders, or pain)
218944-60-6 CAPLUS
Carbamic acid, [[4-{3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2thiazolyl]methyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L7 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 473541-42-3 CAPLUS
CN Carbamic acid,
[[4-(3,5-bie(1,1-dimethylethyl)-4-hydroxyphenyl]-5-methyl-2thiazolyl]methyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

473541-44-5 CAPLUS
Carbamic acid, [[4-[3,5-bis(1,1-dimethylethyl)-4-methoxyphenyl]-2-thiazolyl]methylmethyl-, 1,1-dimethylethyl ester [9CI) (CA INDEX NAME)

473542-72-2 CAPLUS
Carbamic acid, (1-[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2thiazolyl]tehyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

717915-30-5 CAPLUS Glycine, N-[[4-{3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl}-2-thiazoiy]|methyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

717915-34-9 CAPLUS
Glycine, N-[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2thiazolyl]methyl]-N-[(1,1-dimethylethoxy)carbonyl]- (9CI) (CA INDEX

218944-61-7P, 4-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-N-methyl-2-thiazolemethanamine 335242-67-6P, 2,6-Di(tert-butyl)-4-[2-[(methyl)(2-propynyl) amino]methyl]-1,3-thiazol-4-yl]phenol 335242-67-P, 2-[(4-(3,5-Di(tert-butyl)-4-hydroxyphenyl]-1,3-thiazol-2-yl]methyl](methyl) amino]acetonitrile 335242-69-8P, 5-[[(4-(3,5-Di(tert-butyl)-4-hydroxyphenyl)-1,3-thiazol-2-yl]methyl] methyl amino]pentanenitrile 335242-70-1P, 6-[(4-(3,5-Di(tert-butyl)-4-hydroxyphenyl)-1,3-thiazol-2-yl]methyl] (methyl amino]hexanenitrile 335242-71-2P, 2,6-Di(tert-butyl)-4-(2-[(2-hydroxyethyl) (methyl) amino]methyl]-1,3-thiazol-4-yl]phenol 335242-72-3P, 4-[2-([Denzyl(methyl) amino]methyl]-1,3-thiazol-4-yl]phenol 335242-76-7P, 2,6-Di(tert-butyl)-4-[2-[(C-[methyl(4-nitrobenzyl)]mino]methyl]-1,3-thiazol-4-yl]phenol 335242-77-8P,

nitrobenzyl) amino]methyl]-1, 3-thiazol-4-yl]phenol 335242-77-8P,

4-[2-[((4-Aminobenzyl) (methyl) amino]methyl]-1, 3-thiazol-4-yl]-2, 6-di-tert-butylphenol 335242-78-8P, 2,6-Di(tert-butyl)-4-[2-[(4-nitrobenzyl) amino]methyl]-1, 3-thiazol-4-yl]phenol 335242-79-0P,

4-[2-[((4-Aminobenzyl) amino]methyl]-1, 3-thiazol-4-yl]-2,6-di(tert-butyl)phenol 335242-81-4P, 4-[([4-(3,5-Di-tert-butyl)-4-(-4-(i) amino]methyl]-1, 3-thiazol-1-yl]-2,6-di(tert-butyl)phenol 335242-81-8P, 4-[([4-(3,5-Di-tert-butyl)-4-(2-[(3-nitrobenzyl) amino]methyl]-1, 3-thiazol-1-2[([3-nitrobenzyl] amino]methyl]-1, 3-thiazol-4-yl]phenol hydrochloride 335246-05-4P, 4-[2-[(Methylamino]methyl]-1, 3-thiazol-4-yl]phenol hydrochloride 335246-05-4P, 2,6-Di-tert-butyl-4-[2-[(dimethylamino)methyl]-1, 3-thiazol-4-yl]phenol hydrochloride 335246-35-4P, 2,6-Di-tert-butyl-4-[2-[(dimethylamino]methyl]-1, 3-thiazol-4-yl]phenol hydrochloride 335246-35-4P, 2,6-Di-tert-butyl-4-[2-[(dimethylamino]methyl]-1,3-thiazol-4-yl]phenol 335246-35-4P, 2,6-Di-tert-butyl-4-[2-[(dimethylamino)methyl]-1,3-thiazol-4-yl]phenol 335246-30-4PP, 2,6-Di-tert-butyl-4-[2-[(dimethylamino)methyl]-1,3-thiazol-4-yl]phenol 335246-30-4PP, 2,6-Di-tert-butyl-4-[2-[(dimethylamino)methyl]-1,3-thiazol-4-yl]phenol 335246-30-4PP, 2,6-Di-tert-butyl-4-[2-[(dimethylamino)methyl]-1,3-thiazol-4-yl]phenol 473540-20-4PP 473540-21-5P 473540-24-4PP

L7 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

335242-69-8 CAPLUS
Pentanenitrile, 5-[[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]methylamino]- (9CI) (CA INDEX NAME)

335242-70-1 CAPLUS
Hexanenitrile, 6-{[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methylmethylamino]- (9CI) (CA INDEX NAME)

335242-71-2 CAPLUS Phenol.

2,6-bis(1,1-dimethylethyl)-4-(2-[(2-hydroxyethyl)methylamino]meth yl]-4-thiszolyl]- (9CI) (CA INDEX NAME)

RN 335242-72-3 CAPLUS CN Phenol.

CN Prenol, 2,6-bis(1,1-dimethylethyl)-4-[2-([methyl(phenylmethyl)amino]methyl]-4-thiazolyl)- (9CI) (CA INDEX NAME)

17 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
473540-23-0P 473540-28-2P 473540-30-6P
473540-32-0P 473540-33-9P
473540-38-4P 473540-39-9P
473540-84-P 473540-98-0P
473541-38-1P 473541-313-2P 473541-30-0P
473541-32-1P 473541-33-2P 473541-34-3P
473541-35-4P 473541-35-9P 473541-58-PP
473541-60-5P 473541-58-0P 473541-58-PP
473541-60-5P 473541-58-0P 717915-11-2P
717915-36-1P 717915-72-6P 717915-71-0P
717915-62-3P 717915-72-0P
717915-62-3P 717915-73-0P
717915-62-3P 717915-73-0P
717915-79-2P 717915-73-0P
717915-79-2P 717915-73-0P
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717915-79-2P
717915-79-0P
717915-

335242-67-6 CAPLUS

RN 335242-67-6 CAPLUS
On Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[(methyl-2-propynylamino)methyl]-4thiszolyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{He} \\ \text{HC} \\ \text{ECC} \\ \text{CH}_2 \\ \text{N} \\ \text{CH}_2 \\ \text{N} \\ \text{N} \\ \text{SU} \\ \text{CH}_2 \\ \text{N} \\ \text{OH} \\ \text{OH$$

335242-68-7 CAPLUS
Acetonitrile, [[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]methylamino]- (9CI) (CA INDEX NAME)

L7 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

335242-76-7 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[[methyl](4-ntrophenyl]methyl]amino]methyl]-4-thiazolyl]- (9CI)
(CA INDEX NAME)

RN 335242-77-8 CAPLUS
CN Phenol,
4-[2-[[[(4-aminophenyl)methyl]methylamino]methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{t-Bu} \\ \text{HO} \\ \text{t-Bu} \end{array}$$

335242-78-9 CAPIUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[[{4-nitrophenyl}methyl]amino]methyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

335242-79-0 CAPLUS
Phenol, 4-[2-[[[(4-aminophenyl)methyl]amino]methyl]-4-thiezolyl]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

RN 335242-81-4 CAPLUS
CN Butanenitrile, 4-[[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl)methylamino)- (9CI) (CA INDEX NAME)

RN 335242-82-5 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-([[(3-nitrophenyl)methyl]amino]methyl)-4-thiazolyl]- (9CI) (CA INDEX NAME)

RN 335245-99-3 CAPLUS
CN Phenol, 4-(2-[(methylamino)methyl]-4-thiazolyl]-2,6-bis(1-methylethyl)-,
hydrochloride (9CI) (CA INDEX NAME)

Ox HC

RN 335246-01-0 CAPLUS
CN Phenol, 4-[2-{(methylamino)methyl}-4-thiazolyl}-, hydrochloride (9CI)
(CA INDEX NAME)

L7 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued

RN 473540-20-4 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[2-(methylamino)ethyl]-4-thiazolyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

RN 473540-21-5 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[1-(methylamino)ethyl]-4-thiazolyl)-, monohydrochloride (9CI) (CA INDEX NAME)

• HCI

RN 473540-24-8 CAPLUS
CN Acetamide, N-[(4-[3,5-bis(],1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]- (9C1 INDEX NAME)

RN 473540-25-9 CAPLUS

L7 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

●x HCl

N 335246-05-4 CAPLUS
N Phenol, 4-[2-[(dimethylamino)methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)-, hydrochloride (9CI) (CA INDEX NAME)

6v gc1

RN 335246-31-6 CAPLUS
CN Phenol, 4-[2-[(methylamino)methyl]-4-thiazolyl]-2,6-bis(1-methylethyl)(9C1) (CA INDEX NAME)

RN 335246-32-7 CAPLUS
CN Phenol, 4-[2-[(methylamino)methyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

RN 335246-34-9 CAPLUS
CN Phenol, 4-[2-[(dimethylamino)methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

L7 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN [Continued]
CN Carbamic acid, [[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2thiazolyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 473540-28-2 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-{(phenylamino)methyl}-4-thiazolyl](9C1) (CA INDEX NAME)

RN 473540-30-6 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[5-methyl-2-[(methylamino)methyl]-4-thiazolyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

RN 473540-32-8 CAPLUS
CN Acetamide, N-{[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]-N-methyl- (9CI) (CA INDEX NAME)

L7 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

473540-33-9 CAPLUS
2-Thiazolemethanamine, 4-[3,5-bis(1,1-dimethylethyl)-4-methoxyphenyl]-N-methyl-, monohydrochloride (9C1) (CA INDEX NAME)

● HCl

473540-34-0 CAPLUS

RN 473540-34-0 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[(ethylamino)methyl]-4-thiazolyl], monohydrochloride (9CI) (CA INDEX NAME)

● HCl

473540-30-4 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[{(1-methylethyl)amino]methyl}-4-thiazolyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

473540-39-5 CAPLUS
Phenol, 4-{2-{(cyclohexylamino)methyl]-4-thiaxolyl]-2,6-bis(1,1-dimethylethyl)-,monohydrochloride (9C1) (CA INDEX NAME)

ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

● HC1

473541-07-0 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[[[phenylmethyl]amino]methyl]-4-thiazolyl]-, monohydrochloride [9CI] (CA INDEX NAME)

● HCl

473541-32-1 CAPLUS
Carbamic acid, [{4-{3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl}-2-thiazolyl]methyl}-, methyl ester (9CI) (CA INDEX NAME)

473541-33-2 CAPLUS Benzamide, N-[[4-13,5-bis[1,1-dimethylethyl]-4-hydroxyphenyl]-2-thiazolyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{ } \\ \text{ } \\ \text{Ph-C-NH-CH}_2 \\ \text{ } \\ \text{ }$$

ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

● HC1

473540-68-0 CAPLUS

CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[(propylamino)methyl]-4-thiazolyl], monohydrochloride (9CI) (CA INDEX NAME)

● HCl

473540-86-2 CAPLUS

NN 4/30402 44500
NPhenol,
4-[2-{(butylamino)methyl}-4-thiezolyl]-2,6-bis(1,1-dimethylethyl), monohydrochloride (9CI) (CA INDEX NAME)

● HC1

RN 473540-96-4 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-(2-[2-methyl-1-(methylamino)propyl]-4thiazolyl]-, monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) 473541-34-3 CAPLUS Benzeneacetamide, N-[(4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl)- (9CI) (CA INDEX NAME)

473541-35-4 CAPLUS
Propenamide, N-[14-13,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2thiazolyl]methylj- (9C1) (CA INDEX NAME)

473541-50-3 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-(2-[2-(methylamino)ethyl]-4thiezolyl]- (9CI) (CA INDEX NAME)

473541-51-4 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-(2-(1-(methylamino)ethyl)-4-thiazolyl)-(SCI) (CA INDEX NAME)

473541-53-6 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-(5-methyl-2-((methylamino)methyl)-4-thiazolyl)- (GCI INDEX NAME)

473541-55-8 CAPLUS
2-Thiazolemethanamine, 4-(3,5-bis(1,1-dimethylethyl)-4-methoxyphenyl]-N-methyl- (9CI) (CA INDEX NAME)

RN 473541-56-9 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[(ethylamino)methyl]-4-thiazolyl](9CI) (CA INDEX NAME)

473541-60-5 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-{{(1-methylethyl)amino}methyl}-4-thiazolyl}- (9CI) (CA INDEX NAME)

473541-61-6 CAPLUS
Phenol, 4-[2-((cyclohexylamino)methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

717915-19-0 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[(1S)-1-(methylamino)ethyl]-4thiazolyl]-, monohydrochloride (9CI) (CA INDEX NAME)

717915-23-6 CAPLUS Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[(1R)-1-{methylamino}ethyl]-4-thiazolyl]- (CA INDEX NAME)

Absolute stereochemistry.

717915-32-7 CAPLUS
Glycine, N-[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2thiazolyl]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

L7 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN

(Continued)

RN 473541-80-9 CAPLUS CN Phenol, 4-[2-{(butylamino)methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)-(9CI) (CA INDEX NAME)

RN 473541-82-1 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[2-methyl-1-(methylamino)propyl]-4thiazolyl]- (9CI) (CA INDEX NAME)

473541-85-4 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[[(phenylmethyl)amino]methyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

RN 717915-11-2 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[3-methyl-1-(methylamino)butyl]-4thiazolyl]-, monohydrochloride (9CI) (CA INDEX NAME)

L7 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

● HC1

717915-36-1 CAPLUS
Glycine, N-[(4-(3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2thiazolyl]methyl|- (9CI) (CA INDEX NAME)

717915-49-6 CAPLUS

CN Phenol, 4-[2-[(IR)-l-aminoethyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

717915-51-0 CAPLUS

4-[2-[(1S)-1-aminoethyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)-,
monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

• HC1

717915-62-3 CAPLUS
Glycine, N-{[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolylimethyl]-N-(2-ethoxy-2-oxoethyl)-, ethyl ester, hydrochloride
(9CI) (CA INDEX NAME)

● HC1

RN 717915-74-7 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[3-methyl-1-(methylamino)butyl]-4thiazolyl]- (9CI) (CA INDEX NAME) 717915-74-7 CAPLUS

717915-77-0 CAPLUS Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[(1S)-1-(methylamino)ethyl]-4-thiazolyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) L7 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

717915-79-2 CAPLUS Glycine, N-[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]-, ethyl ester (9CI) (CA INDEX NAME)

717915-85-0 CAPLUS Phenol, 4-[2-[(1R)-1-aminosthyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

717915-86-1 CAPLUS
Phenol, 4-[2-[(1S)-1-aminoethyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L7 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:981469 CAPLUS
TITLE: Phenolic thiazoles as novel orally-active neuroprotective agents.

AUTHOR(S): Harnett, Jeremiah J.: Roubert, Veronique; Dolo, Christine; Charnet, Christelle; Spinnewyn, Brigitte; Cornet, Sylvie; Rolland, Alain; Marin, Jean-Gregoire; Bigg, Dennis; Chabrier; Pierre-E.

CORPORATE SOURCE: Types Research Laboratories, Department of Medicinal Chemistry, Institute Henri Beaufour, Les Ulis, 91966, Fr.

Chemistry, Institute Henri Beaurour, Les Ulis, 9 Fr. Bioorganic & Medicinal Chemistry Letters (2004), 14(1), 157-160 CODEN: BMCLE8; ISSN: 0960-894X Elsevier Science B.V. Journal

SOURCE:

PUBLISHER:

DOCUMENT TYPE: LANGUAGE:

English CASREACT 140:199246 OTHER SOURCE(S):

Phenolic thiazoles I (R = H, Me) were prepared and tested in vivo for antioxidant and neuroprotective activities. I showed potent antioxidant activity and potent neuroprotection in mitochondrial toxin models. Furthermore, I also possessed good oral bioavailability. 663172-98-39 RI: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation, antioxidant, and neuroprotective activity of (aminomethyl) (hydroxyaryl)thiazole salts via sulfurization of aminoacetamides followed by heterocyclization with di(t-butyl)hydroxyphenacyl bromide, deprotection, and salt formation) 663172-95-0 CAPLUS Phenol, 4-{2-(aminomethyl)-4-thiazolyl)-2,6-bis(1,1-dimethylethyl)-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HCl

RN 663172-98-3 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[(methylamino)methyl]-4-thiazolyl], dihydrochloride (9CI) (CA INDEX NAME)

●2 HC1

218944-60-6P 218944-61-7P 335242-74-5P 335242-75-6P

335242-75-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation, antioxidant, and neuroprotective activity of (aminomethy)) (hydroxyaryl]thiazole salts via sulfurization of aminoacetamides followed by heterocyclization with ditbutyl)hydroxyphenacyl bromide, deprotection, and salt formation) 218944-60-6 CAPLUS

Carbamic acid, [[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

218944-61-7 CAPLUS

CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-{2-{(methylamino)methyl}-4-thiazolyl}-{9C1} (CA INDEX NAME)

L7 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:319488 CAPLUS
DOCUMENT NUMBER: 138:337988
TITLE: Novel 2-[(iminomethyl)amino]phenyl derivatives useful as inhibitors of No synthase and lipid peroxidation, their preparation, their application as medicines,

pharmaceutical compositions containing them Chabrier De Lassauniere, Pierre Etienne; Auvin, INVENTOR (S):

PATENT ASSIGNEE(S):

Bigg, Dennis; Auguet, Michel; Harnett, Jeremiah Societe de Conseils de Recherches et D'Applications acientifiques (S.C.R.A.S.), Fr. U.S. Pat. Appl. Publ., 78 pp., Cont.-in-part of U.S. Ser. No. 882,264. CODEN: USXXCO Patent English 4 SOURCE:

DOCUMENT TYPE:

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

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										PR 1	997-	7701		1	A 1	9970	620
									1	WO I	998-	FR28	В	,	v 1	9980	216
									,	WO I	998-	FR12:	50	,	v 1	9980	615

335242-74-5 CAPLUS
Carbamic acid, [4-(3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2thiazoiyllmethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

ANSWER 6 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN

335242-75-6 CAPLUS
Phenol, 4-[2-(aminomethyl)-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI)
(CA INDEX NAME)

REFERENCE COUNT:

22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L7 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN US 2001-882264 (Continued) A2 20010615

US 1999-381749 A2 19990922 US 2002-191950 A3 20020709

US 2004-898916 A3 20040726

OTHER SOURCE(S):

MARPAT 138:337988

Title compds., e.g., N-[4-[[[[4-(3,5-di-tert-butyl-4-hydroxyphenyl]-1,3-thiazol-2-yl]methyl]aminolmethyl]phenyl]thiophene-2-carboximidamide [I] are prepared The compds. are inhibitors of NO synthases, and are also antioxidants which inhibit lipid peroxidn. Approx. 70 examples are

prepared

I had IC50 for inhibiting rat neuronal NO synthase in vitro < 3.5 µM,
and the IC50 for inhibiting rat cerebral lipid peroxidn. in vitro is < 30

and the 1630 for finite fing (at Cetebral Tipla peroxida. In Vitro 1, pm. 515915-18-69, N-[4-[[[4-(3,5-Di-tert-butyl-4-hydroxyphenyl)-1,3-thiazol-2-yl]methyl]amino]methyl]phenyl]thiophene-2-carboximidamide 515915-19-79, N-[3-{[[(4-(3,5-Di-tert-butyl-4-hydroxyphenyl)-1,3-thiazol-2-yl]methyl]amino]methyl]phenyl]thiophene-2-carboximidamide 515915-20-09, N-[4-{[[[4-(3,5-Di-tert-butyl-4-hydroxyphenyl]-1,3-thiazol-2-yl]methyl](methyl)amino]methyl]phenyl]thiophene-2-carboximidamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(preparation and testing of 2-{(iminomethyl)amino)phenyl derivs. as inhibitors of NO synthase and lipid peroxidn.)
515815-18-6 CAPLUS
2-Thiophenecarboximidamide, N-[4-[([4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]amino]methyl]phenyl]- (9CI) (CA INDEX NAME)

515815-19-7 CAPLUS 2-Thiophenecarboximidamide, N-[3-[[[[4-[3,5-bis(1,1-dimethylethyl)-4-

ANSWER 7 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) hydroxyphenyl]-2-thiazolyl]methyl]amino]methyl]phenyl]- (9CI) (CA INDEX NAWE)

515815-20-0 CAPLUS
2-Thiophenecarboximidamide, N-[4-[{[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]methylamino]methyl]phenyl]- (9CI) (CA INDEX NAME) RN CN

218944-60-6P, 4-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-N[(1,1-dimethylethoxy)carbonyl]-N-methyl-2-thiazolemethanamine
218944-61-7P, 4-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-Nmethyl-2-thiazolemethanamine 335242-74-8P, Benzyl
[4-[3,5-di(tert-butyl)-4-hydroxyphenyl]-1,3-thiazol-2-yl]methylcarbamate
335242-75-6P, 4-[2-(Aminomethyl]-1,3-thiazol-4-yl]-2,6-(di-tertbutyl)phenol 335242-76-7P, 2,6-Di-tert-butyl-4-[2-(Imethyl)4nitrobenzyl)amino]methyl]-1,3-thiazol-4-yl]phenol 335242-77-8P,

4-[2-[{(4-Aminobenzyl) (methyl) amino]methyl]-1,3-thiazol-4-yl}-2,6-di-tert-butylphenol 335242-78-89, 2,6-Di-tert-butyl-4-[2-{[(4-Aminobenzyl) amino]methyl]-1,3-thiazol-4-yl]phenol 335242-79-0P, 4-[2-{((4-Aminobenzyl) amino]methyl]-1,3-thiazol-4-yl]-2,6-di-tert-butylphenol RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and testing of 2-{(iminomethyl)amino]phenyl derivs. as inhibitors of NO synthase and lipid peroxidn.)

RN 218944-60-6 CAPLUS
CN Carbamic acid, [[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]methyl-, 1,1-dimethylethyl ester (SCI) (CA INDEX NAME)

ANSWER 7 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN Phenol, (Continued)

335242-78-9 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-(2-({(4-nitrophenyl)methyl]amino|methyl]-4-thiazolyl|- (9CI) (CA INDEX NAME)

335242-79-0 CAPLUS
Phenol, 4-[2-[[(4-aminophenyl)methyl]amino]methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

L7 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

218944-61-7 CAPLUS

CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[(methylamino)methyl]-4-thiazolyl][9C1 (CA INDEX NAME)

335242-74-5 CAPLUS
Carbamic acid, [[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

335242-75-6 CAPLUS
Phenol, 4-[2-(aminomethyl)-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI)
(CA INDEX NAME)

335242-76-7 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[[methyl](4-nitrophenyl]methyl]amino]methyl]-4-thiazolyl)- (9CI (CA INDEX NAME)

$$\begin{array}{c} \text{t-Bu} \\ \text{HO} \\ \text{t-Bu} \end{array}$$

335242-77-8 CAPLUS

L7 ANSWER 8 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:97298 CAPLUS
DOCUMENT NUMBER: 138:131175
Use of thiazole derivatives for preparing a medicine for protecting mitochondria August Michel; Chabrier De Lassauniere, Pierre-Etienne: Harnett, Jeremitah
Societe De Conseils De Recherches Et D'Applications Scientifiques (S.C.R.A.S.), Fr.
SOURCE: PTXND2
DOCUMENT TYPE: Patent
LANGUAGE: French

LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

					KIND DATE							DATE					
PA	TENT I	NO.			KIN	D	DATE		- 4	APPL	ICAT	ION	NO.		D	ATE	
WO	2003																
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							DK,										
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							MD,										
		PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	sĸ,	SL,	ТJ,	TM,	TN,	TR,	TT,	TZ,
		UA,	UG,	US,	UŹ,	VN,	YU,	ZA,	ZM,	ZW							
	RW:	GH,	GM,	KE,	LS,	MW.	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AT,	Β£,	BG,
							EE,										
		PT,	SE,	SK,	TR,	BF.	ВJ,	CF.	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,
					TG			-	-	-							
FR	2827	772	-		A1		2003	0131		FR 2	001-	9979			2	0010	726
FR	2827	772			B1		2006	0428									
CA	2455	635			AA		2003	0206		CA 2	002-	2455	635		2	0020	725
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							RO,										
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									20 2	002-	FR26	60			102n	725	
															-		

OTHER SOURCE(S):

MARPAT 138:131175

The invention discloses compds. I [A = Q1, Q2; R5 = H, alkyl; R6-R8 = H, alkyl, cycloalkyl, OH, alkoxy; R11 = H, alkyl; R9, R10, R12 = H, alkyl, OH, alkoxy; B = H, alkyl; n = 0-5; R1, R2 = H, alkyl, cycloalkyl; R3, R4

(Continued)

OH, alkoxy; B = H, alkyl; n = 0-5; Rl, RZ = H, alkyl, cycloalkyl; R3, R4

H, alkyl, or R3NR4 form (un)substituted heterocycle comprising in all 2 heteroatoms and 5-7 members]. The compds. can be used for preparing a medicine for protecting mitochondria, and in particular a medicine for preventing or treating cirrhosis.

IT 218944-61-7 335242-73-6 473341-51-6

R1: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(thiazole derivs. for preparing a medicine for protecting mitochondria)

RN 218944-61-7 CAPLUS

CN Phenol,

2,6-bis(1,1-dimethylethyl)-4-[2-{(methylamino)methyl}-4-thiazolyl]-(9CI) (CA INDEX NAME)

335242-75-6 CAPLUS
Phenol, 4-[2-(aminomethyl)-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI)
(CA INDEX NAME)

L7 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2006 ACS ON STN ACCESSION NUMBER: 2002:814116 CAPLUS DOCUMENT NUMBER: 137:325417

Preparation and application of 5-membered TITLE:

heterocycles

as medicaments

INVENTOR(S):

PATENT ASSIGNEE (S):

as medicaments
Harnett, Jeremiah; Bigg, Dennis; Liberatore,
Anne-Marie; Rolland, Alain
Societe De Conseils De Recherches Et D'applications
Scientifiques (SCRAS), Fr.
PCT Int. Appl., 132 pp.
CODEN: PIXXD2 SOURCE:

DOCUMENT TYPE: Patent French

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

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			PI.	PT.	RO.	RU.	SD.	SE.	SG.	SI.	SK.	SL	T.1.	TM	TN.	TR	TT.	TZ
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		RW:										TZ.	UG.	ZM.	ZW.	AT.	BE,	CH.
			CY.	DE.	DK.	ES.	FI.	FR.	GB.	GR.	IE.	IT.	LU.	MC.	NL.	PT	SE,	TR.
			BF.	BJ.	CF.	CG.	CI.	CM.	GA.	GN.	GO.	GW.	MI.	MR.	NE.	SN	TD.	TG
	FR	2823 2823 2443 1379	208			A1		2002	1011		FR 2	2001-	4943				20010	410
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	CA	2443	103			AA		2002	1024		CA 2	2002-	2443	403		:	20020	409
	EΡ	1379	514			A2		2004	0114		EP 2	2002-	7619	21		- 2	20020	409
		R:	AT,	BE,	CH,	DΕ,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR						
	CN	1535	267			A		2004	1006		CN 2	2002-	8079	37		- 2	20020	409
	JΡ	2004	5315	26		T2		2004	1014		JP 2	2002-	5814	12		- 2	10020	409
	ΝZ	5286	45			А		2004	1126		NZ 2	002-	5286	45		- 2	10020	409
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	ZA	2003	0077	50		А		2004	0726		ZA 2	2003-	7750			- 2	:0031	003
-	МО	2003	0045	24		А		2003	1029	1	NO 2	2003-	4524			- 2	:0031	009
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											FR 2	002-	1811		2	A 2	20020	214
											FR 1	999-	1264	3	1	A 1	19991	011
											FR 2	000-	1015	1	1	A 2	0000	801
											FR 2	000-	1116	9	,	A 2	0000	901
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																	0020	
										1	WO 2	002-	FR12:	18	,	4 2	0020	409
											J\$ 2	003-	68100	02	1	12 2	0031	008

ANSWER 8 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

473541-51-CAPLUS q:suq:=9:14 CAPLUS Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[1-(methylamino)ethyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 9 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

The invention relates to thiszole, oxazole or imidazole derivs. having at least one of the following pharmacol. activities:: inhibition of

11

monoamine
oxydases (MAO); inhibition of lipid peroxidn.; modulation of sodium
channels. The inventive compds. comprise, for example,
2,6-di(tert-butyl)-4-(2-[2-(methylamino)ethyl]-1,3-thiazol-4-yl)phenol
(I); and 4-methylpentyl 2-[4-(1,1'-biphenyl-4-yl)-1H-imidazol-2-yl]ethyl
carbamate (II). Thus, I-HCl was prepared from N-methyl-Balaninenitrile via. N-protection with (Boc)20 in CH2Cl2 containing
EtN(CHMe2)2, sulfurization with H2S in EtOH containing EtN,
cyclocondensation
with g-bromo-1-13.5-di(fest-butyl) 4-brows-1-13.5-di(fest-butyl) 4

ocondensation with α-bromon-1-{3,5-di(tert-butyl)-4-hydroxyphenyl]ethanone and acid-catalyzed deprotection with HCl in EtOAc. By virtue of their pharmacol, properties, said compds. can be used to treat one of the following disorders or diseases: Parkinson's disease, senile dementia, Alzheimer's disease, Huntington's chorea, ampotrophic lateral sclerosis, schizophrenia, depression, psychoses, migraine or pain, especially

schizoparenia, depression, psychoses, migraine or pain, especially neuropath.

pain. The pharmacol. activity of I was determined [CISO ≤ 10 μM vs. monoamine oxydase B; CISO ≤ 10 μM vs. lipid peroxidn.; CISO ≤ 1.0 μM on sodium channels from the cerebral cortex of rate].

IT 473541-69-49

IT 473541-69-4P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of 5-membered heterocycles with one of the following pharmacol.

ANSWER 9 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) activities: monoamine oxydase inhibition, lipid peroxydation or sodium channel modulation)

473541-69-4 CAPLUS

RN 4/3041-0574 Galler (CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[(propylamino)methyl]-4-thiazolyl]-(9CI) (CA INDEX NAME)

473540-20-4P 473540-21-5P 473540-24-8P 473540-25-9P 473540-25-9P 473540-28-P 473540-29-3P 473540-32-8P 473540-31-8P 473540-31-8P 473540-31-8P 473540-31-8P 473540-31-8P 473540-31-8P 473540-31-8P 473540-31-8P 473540-31-8P 473541-31-2P 473541-31-2P 473541-31-4P 473541-31-4P 473541-31-8P 473541-31-31-8P 473541-31-31-8P 473541-31-31-31-8P 473541-31-31-8P 473541-31-31-8P 473541-31-31-31-31-8P 47354

(preparation of 5-membered heterocycles with one of the following macol.

macol.
activities: monoamine oxydase inhibition, lipid peroxydation or sodium
 channel modulation)
473540-20-4 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[2-(methylamino)ethyl]-4thiazolyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● RC1

473540-21-5 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[1-(methylamino)ethyl]-4-thiazolyl]-, monohydrochloride (9CI) (CA INDEX NAME)

L7 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

473540-30-6 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[5-methyl-2-[(methylamino)methyl]-4-thiazoiyl)-, monohydrochloride (9CI) (CA INDEX NAME)

473540-32-8 CAPLUS Acetamide, N-[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]-N-methyl- (9CI) (CA INDEX NAME)

473540-33-9 CAPLUS
2-Thiazolemethanamine, 4-[3,5-bis{1,1-dimethylethyl}-4-methoxyphenyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

ANSWER 9 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

● HC1

473540-24-8 CAPLUS
Acetamide, N-[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl)- (9CI) (CA INDEX NAME)

473540-25-9 CAPLUS Carbamic acid, [[4-[3,5-bis(],1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]-, ethyl ester (9CI) (CA IMDEX NAME)

RN 473540-28-2 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[(phenylamino)methyl]-4-thiazolyl](9C1) (CA INDEX NAME)

473540-29-3 CAPLUS
Phenol, 4-[2-[[[2-(dimethylamino)ethyl]methylamino]methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

L7 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

473540-34-0 CAPLUS RN

2,6-bis(1,1-dimethylethyl)-4-[2-[(ethylamino)methyl]-4-thiazolyl], monohydrochloride (9CI) (CA INDEX NAME)

• HC1

473540-38-4 CAPLUS
Phenol, 2,6-bis(),1-dimethylethyl)-4-[2-[[(1-methylethyl)amino]methyl]-4-thiazolyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

473540-39-5 CAPLUS
Phenol, 4-[2-[(cyclohexylamino)methyl)-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HC1

RN 473540-68-0 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[(propylamino)methyl]-4-thiazolyl], monohydrochloride (9CI) (CA INDEX NAME)

● HC1

RN 473540-86-2 CAPLUS
CN Phenol,
4-[2-[(butylamino)methyl)-4-thiazolyl]-2,6-bis(1,1-dimethylethyl), monohydrochloride (9CI) (CA INDEX NAME)

● HC1

RN 473540-96-4 CAPLUS
CN Phenol,
2,6-bis[1,1-dimethylethyl)-4-[2-{2-methyl-1-(methylamino)propyl}-4thiazolyl]-, monohydrochloride (9CI) (CA INDEX NAME)

■ HC1

473541-07-0 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-{{(phenylmethyl)amino}methyl}-4-thiazolyl]-, monohydrochloride (9CI) (CA INDEX NAME)

ANSWER 9 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

473541-50-3 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[2-{methylamino}ethyl}-4-thiazolyl]- (GC INDEX NAME)

MeNH-CH2-CH2

473541-51-4 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[1-(methylamino)ethyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

473541-53-6 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-{5-methyl-2-[(methylamino)methyl]-4-thiazolyl}- (9CI) (CA INDEX NAME)

473541-55-8 CAPLUS
2-Thiazolemethanamine, 4-[3,5-bis(1,1-dimethylethyl)-4-methoxyphenyl]-N-methyl- (9CI) (CA INDEX NAME)

• HC1

473541-32-1 CAPLUS
Carbamic acid, [{4-{3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl}-2-thiazolyl]methyl}-, methyl ester (9CI) (CA INDEX NAME)

473541-33-2 CAPLUS
Benzamide, N-[(14-3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl)-2-thiazolyljmethyl)- (9CI) (CA INDEX NAME) RN CN

$$\begin{array}{c} \text{OH} \\ \text{Ph-C-NH-CH}_2 \\ \text{S} \end{array} \begin{array}{c} \text{OH} \\ \text{Bu-t} \end{array}$$

473541-34-3 CAPLUS
Benzeneacetamide, N-{{4-{3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl}-2-thiazolyl]methyl]- (9CI) (CA INDEX NAME)

473541-35-4 CAPLUS
Propanamide, N-[[4-13,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]- (9CI) (CA INDEX NAME)

L7 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 473541-56-9 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[(ethylamino)methyl]-4-thiazolyl](SCI) (CA INDEX NAME)

473541-60-5 CAPLUS
Phenol, 2, 6-bis(1, 1-dimethylethyl)-4-{2-[[(1-methylethyl)amino]methyl]-4-thiazolyl]- (9C1) (CA INDEX NAME)

473541-61-6 CAPLUS
Phenol, 4-[2-[(cyclohexylamino)methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

RN 473541-80-9 CAPLUS
CN Phenol,
4-[2-[(butylamino)methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl){9CI} (CA INDEX NAME)

RN 473541-82-1 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[2-methyl-1-(methylamino)propyl]-4thiazolyl]- (9CI) (CA INDEX NAME)

473541-85-4 CAPLUS
Phenol, 2.6-bis(1,1-dimethylethyl)-4-(2-[[(phenylmethyl)amino]methyl]-4-thiazolyl]- (SCI) (CA INDEX NAME)

IT 218944-60-6F 335242-74-5P 335242-75-6P
473541-38-7P 473541-41-2P 473541-42-3P
473541-44-5P 473542-72-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation of 5-membered heterocycles with one of the following pharmacol.

macol.
 activities: monoamine oxydase inhibition, lipid peroxydation or sodium
 channel modulation)
218944-60-6 CAPLUS
Carbamic acid, [[4-[3,5-bis[1,1-dimethylethyl)-4-hydroxyphenyl]-2thiazolyl]methyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

ANSWER 9 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

● HC1

473541-42-3 CAPLUS
Carbamic acid,
-[3,5-bia[1,1-dimethylethyl]-4-hydroxyphenyl]-5-methyl-2thiazolyl]methyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

473541-44-5 CAPLUS
Carbamic acid, [[4-{3,5-bis{1,1-dimethylethyl}-4-methoxyphenyl}-2-thiazolyl]methyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

473542-72-2 CAPLUS
Carbamic acid, [1-[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]ethyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA.INDEX NAME)

L7 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

335242-74-5 CAPLUS
Carbamic acid, [{4-{3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl}-2-thiazolyl]methyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

335242-75-6 CAPLUS
Phenol, 4-[2-(aminomethyl)-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI)
(CA INDEX NAME)

473541-38-7 CAPLUS
Carbamic acid, {2-{4-{3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl}-2-thiazolyl}ethyl}methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 473541-41-2 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[{methylamino}methyl]-4-thiazolyl], monohydrochloride (9CI) (CA INDEX NAME)

L7 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L7 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:6385 CAPLUS
DOCUMENT NUMBER: 136:69731
TITLE: 136:69731
Preparation of N-phenylthiophenecarboxamidines and analogs as No synthase and lipid peroxidation inhibitors
INVENTOR(S): Chabrier de Lassauniere, Pierre Etienne; Auvin,

INVENTOR (S): Serge;

PATENT ASSIGNEE(S):

Bigg, Dennis; Auguet, Michel; Harnett, Jeremiah Societe de Conseils de Recherches et d'Applications Scientifiques (S.C.R.A.S.), Fr. U.S., 63 pp., Cont.-in-part of U. S. Ser. No.

CODEN: USXXAM Patent English 4 DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT	TENT				KIN		DATE					TION			,	DATE	
US	6335	445										-4562				19991	207
	2761				B1 A1		1998	0925		FR	1997	-3528			- 3	9970	
	2761				B1		2000										
FR	2764	889			A1		1998	1224		FR	1997	-7701			:	19970	620
FR	2764	889			B1		2000	0901				-7701					
WO	9842	696										-FR28				19980	216
	W:	AL.	AM.	AT.	AU,	AZ.	BA,	BB,	BG,	BF	, BY	, CA,	CH,	CN,	CU,	CZ.	DE,
		DK.	EE.	ES.	FI.	GB.	GE.	GH.	GH,	GW	, KU	, ID,	IL.	IS,	JP.	KE.	KG,
		KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	L	, LV	, MD,	MG,	MK,	MN,	MW,	MX,
		NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG	, si	, sk,	SL,	TJ,	TM.	TR,	TT,
		UA,	UG,	US,	UZ,	٧N,	YU,	ZW									
	RW:	GH,	GM,	KE,	LS,	MW,	SD,	SZ,	UG,	24	, AT	, BE,	CH,	DE,	DK.	ES,	FI,
										P1	, SE	, BF,	ВJ,	CF,	CG,	CI,	CM,
							SN,										
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US	2002 6630 2002	461			B2		2003	1007									
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										WO	1998	-FR28	8		w :	9980	216
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ANSWER 10 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L7 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
US 2004-898916 A3 20040726

OTHER SOURCE(S): MARPAT 136:69731

RZZ1ZZZ3N:C(NH2)R1 [I; R = H, (un)substituted C6H4OR3, indoly1, etc.; R1 alkyl or (un)substituted (hetero)aryl; R3 = H, alkyl, etc.; Z = bond, CO, alkylene(carbonyl), CONH, etc.; Z1 = bond or heterocyclylene; Z2 = bond, alkylene(coxy), etc.; Z3 = (un)substituted phenylene] were prepared Thus, 4-(O2N)C6H4NH2 was amidated by 3,5-di-tert-butyl-4-hydroxybenzoic acid

the reduced product amidated by S-methyl-2-thiophenethiocarboximide hydroiodide to give title compound II. Data for biol. activity of I were given.

IT 218944-60-69 218944-61-79
RL: RCT (Reactant); SFN (Synthetic preparation); FREP (Preparation); RACT (Reactant or reagent) (preparation of N-phenylthiophenecarboxamidines and analogs as NO synthese and lipid peroxidn. inhibitors)
RN 218944-60-6 CAPLUS
CC Carbamic acid, [[4-{3,5-bis{1,1-dimethylethyl}-4-hydroxyphenyl}-2-thiazolyl]methyl]methyl-, 1,1-dimethylethyl ester (SCI) (CA INDEX NAME)

218944-61-7 CAPLUS

RN 218944-61-7 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[{methylamino}methyl]-4-thiazolyl]{9CI} (CA INDEX NAME)

L7 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN ACCESSION NUMBER: 2001:283789 CAPLUS DOCUMENT NUMBER: 134:311210

134:311210 5-Membered heterocycle derivatives useful as TITLE:

monoamine oxidase inhibitors, lipid peroxidation inhibitors,

and sodium channel modulators, and the production

thereof.

and use thereof as medicaments
Chabrier de Lassauniere, Pierre-Etienne; Harnett,
Jeremiah; Bigg, Dennis; Pommier, Jacques; Lannoy,
Jacques; Liberatore, Anne-Marie: Thurieau, Christophe
Societe de Conseils de Recherches et d'Applications
Scientifiques (S.C.R.A.S, Fr.
PCT Int. Appl., 261 pp.
CODEN: PIXXD2
Patent
French
4 INVENTOR (S):

PATENT ASSIGNEE (S):

SOURCE:

DOCUMENT TYPE:

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA'	TENT	NO.								APPLICATION NO.								
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WO	2001						2002											
	W:						ΑU,											
							DM,											
							JP,											
							MK,											
					SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UΑ,	UG,	US,	υz,	V	
			ZA,															
	RW:																	
							GB,								SE,	BF,	В	
			CG,	CI,	CN,	GΑ,	GN,	G₩,	ML,	MR,	ΝE,	SN,	TD,	TG				
	2799				A1		2001	0413		FR 1	999-	1264	3		1	9991	01	
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CA 2388505					AA		2001	0419		CA 2	000-	2388	505		2	0001	01	
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	R:						ES,					LI,	LU,	NL,	SE,	MC,	P	
		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL								
ΕP	1228	760			A2		2002	0807		EP 2	002-	7676	3		2	0001	01	
ΕP	1228	760			A.3		2004	0128										
	R:						ES,				IT,	LI,	LU,	NL,	SE,	KC,	P	
		IE,	SI,	LT,	LV,	FI,	RO,	MК,	CY,	AL								
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NZ	5183	04			A		2004	0730		NZ 2	000-	5183	04		2	0001	01	
NZ	5334	29			A		2004	0924		NZ 2	000-	5334	29		2	0001	01	
ΑU	5183 5334 7831 1589	29			B2		2005	0929		AU 2	000-	7796	5		2	0001	01	
EΡ	1589	007			A2		2005	1026		EP 2	005-	7674	9		2	0001	01	
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	P	
							CY											
	2271						2006											
NO	2002	0016	89		A		2002	0530		NO 2	002-	1689			2	0020	41	
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										FR 2	-000	1015	1		A 2	0000	80	

L7	ANSWER	11	OF	18	CAPLUS	COPYRIGHT		CS on STN 2000-11169	(Conti	nued) 20000901
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							WO	2000-FR2805	W	20001010
							FR	2001-4943	A	20010410
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							us	2002-89993	A2	20020404
							WO	2002-FR1218	A1	20020409
							us	2003-681002	A2	20031008

OTHER SOURCE(S): MARPAT 134:311210

The invention relates to pharmaceutical use of heterocyclic compds. of general formula $\operatorname{Het}(A)$ (B) $-(\operatorname{GR2}) - \operatorname{GR1R2} - \mathbb Q$ []; wherein the substituted heterocyclic ring $\operatorname{Het}(A)$ (B) $= \mathbb Q - \mathbb Q + \mathbb Q$; a various arely or heteroaryl systems, especially a substituted Ph or biphenyl radical, or also alkyl, cycloalkyl, or cycloalkyl, $\mathbb Q$ especially H or alkyl, or raiso aryl

or substituted alkyl; X = especially NH or S, or also substituted NH; Y = O or S; n = 0-6; R1, R2 = especially H, alkyl, or cycloslkyl; Q = NR3R4 or OR5; R3 and R4

ANSWER 11 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

335242-76-7 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[[methyl](4-ntrophenyl)methyl]amino|methyl]-4-thiazolyl]- (SCI) (CA INDEX NAME)

335242-78-9 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-[2-[[[(4-ntrophenyl)methyl]mino]methyl]-4-thiazolyl](CA INDEX NAME)

335242-67-6P, 2,6-Di(tert-butyl)-4-[2-[[methyl [2-propynyl] amino]methyl]-1,3-thiazol-4-yl]phenol 335242-68-7P, 2-[[4-[3,5-D](tert-butyl]-4-hydroxyphenyl]-1,3-thiazol-2-yl]methyl](methyl]maino]acetonitrile 335242-69-6P, 5-[[4-[3,5-D](tert-butyl]-4-hydroxyphenyl]-1,3-thiazol-2-yl]methyl](methyl)amino]pentanentrile 335242-70-1P, 6-[[4-[3,5-D](tert-butyl]-4-hydroxyphenyl]-1,3-thiazol-2-yl]methyl](methyl)amino]hexanenitrile 335242-71-2P, 2,6-Di(tert-butyl]-4-[2-[[(2-hydroxyethyl)(methyl)amino]methyl]-1,3-thiazol-4-yl]phenol 335242-72-3P, 4-[2-[[(4-minobenzyl](methyl)amino]methyl]-1,3-thiazol-4-yl]-2,6-di(tert-butyl)phenol 335242-77-6P, 4-[2-[[(4-minobenzyl)(methyl)amino]methyl]-1,3-thiazol-4-yl]-2,6-di(tert-butyl)phenol 335242-79-0P, 4-[2-[[(4-minobenzyl)amino]methyl]-1,3-thiazol-4-yl]-2,6-di(tert-butyl)phenol 335242-0P-0P, 4-[2-[[(4-minobenzyl)amino]methyl]-1,3-thiazol-4-yl]-2,6-di(tert-butyl-4-hydroxyphenyl)-1,3-thiazol-4-yl]-2,6-di(tert-butyl-4-[2-[[(4-minobenzyl)amino]methyl]-1,3-thiazol-4-yl]phenol 335245-99-3P, 2,6-Di-iaropenzyl-4-[2-[(4-minobenzyl)amino]methyl]-1,3-thiazol-4-yl]phenol 335245-99-3P, 2,6-Di-iaropenzyl-4-[2-[((4-minobenzyl)amino]methyl]-1,3-thiazol-4-yl]phenol 335245-99-3P, 2,6-Di-iaropenzyl-4-[2-[((4-minobenzyl)amino]methyl]-1,3-thiazol-4-yl]phenol 335245-99-3P, 2,6-Di-iaropenzyl-4-[2-[((4-minobenzyl)amino]methyl]-1,3-thiazol-4-yl]phenol hydrochloride

L7 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) = esp. H, alkyl, cycloalkyl, alkynyl, cyanoalkyl alkoxycarbonyl, aralkoxycarbonyl or (cycloalkyl) avycarbonyl R5 = H, alkyl, alkynyl, or cyanoalkyl]. I and their racemates, enantiomers, and/or selts can be

for producing medicaments for inhibiting monomine oxidases (MAO), inhibiting lipid peroxidn., and/or for acting as modulators of sodium channels. The resulting medicaments are particularly for use in treating Parkinson's disease, senile dementia, Alzheimer's disease, Huntington's chorea, amyotrophic lateral sclerosis, schizophrenia, depression, psychosis, pain and epilepsy. Approx. 350 synthetic examples of I and their salts are given, and numerous free bases of I are claimed. For instance, protection of sarcosinamide-HCl with BOC anhydride gave 72% BOC-N(Me)CH2COMH2, which was converted to the thioamide with (P2S5)2 in 65% yield. Cyclocondensation of the thioamide with cond-1-(3,5-di-tetr-butyl-4-hydroxyphenyl)ethanone (28%), followed by deprotection (73%) and salification (92%), gave thiazole deriv. II as the HCl salt. II bited

bited binding of the MAO-B specific ligand [3H]-Ro-19-6327 to rat mitochondrial prepns. with IC50 < 10 µM. Selected I also inhibited formation of malondialdehyde by lipid peroxidn. In rat cerebral cortex prepns., and inhibited specific binding of [3H]-batrachotoxin to voltage-dependent sodium channels in rat cerebral cortex homogenates. 218944-61-7P, 4-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-N-methyl-2-thiazolemethanamine 335242-74-5P, Benzyl

[[4-[3,5-di(tert-butyl)-4-hydroxyphenyl]-1,3-thiazol-2-yl]methyl]carbamate
335242-76-79, 2,6-Di(tert-butyl)-4-[2-[([methyl)(4nttrobenzyl]amino]methyl]-1,3-thiazol-4-yl]phenol 335242-78-99,
2,6-Di(tert-butyl)-4-[2-[([4-nitrobenzyl]amino]methyl]-1,3-thiazol-4yl]phenol
Ri: BaC (Biological activity or effector, except adverse); BSU
(Biological
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)
(drug candidate; preparation of five-membered heterocycle derivs. as

inhibitors, lipid peroxidn. inhibitors, and sodium channel modulators)
RN 218944-61-7 CAPLUS
CN Phenol,
2,6-bis[1,1-dimethylethyl]-4-[2-{(methylamino)methyl}-4-thiazolyl](9CI) (CA INDEX NAME)

335242-74-5 CAPLUS
Carbamic acid, [[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2thiazolyl]methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

ANSWER 11 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) 335246-01-09, 4-[2-[(Methylamino]methyl]-1,3-thiazol-4-yl]phenol hydrochloride 335246-05-49, 2,6-Di-tert-butyl-4-[2-[(dimethylamino]methyl]-1,3-thiazol-4-yl]phenol hydrochloride 335246-19-09, 4-[3,5-Bis[1,1-dimethylethyl]-4-hydroxyphenyl]-N-methyl-2-thiazolemethanamine hydrochloride 335246-31-69, 2,6-Diisopropyl-4-[2-[(methylamino]methyl]-1,3-thiazol-4-yl]phenol 335246-32-79, 4-[2-[(Methylamino]methyl]-1,3-thiazol-4-yl]phenol 335246-34-99, 2,6-Di-tert-butyl-4-[2-[(dimethylamino]methyl]-1,3-thiazol-4-yl]phenol 345246-34-99, 2,6-Di-tert-butyl-4-[2-[(dimethylamino]methyl]-1,3-thiazol-4-yl]phenol

thiazol-4-yl]phenol RL: BAC (Biological activity or effector, except adverse); BSU

RI: BAC (Biological activity of climate (Biological) (Biological) study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (drug candidate; prepn. of five-membered heterocycle derivs. as MAO inhibitors, lipid peroxidn. inhibitors, and sodium channel modulators) RN 335242-67-6 CAPLUS

NN 3332427676 GPD03
CN Pheno;
2,6-big[1,1-dimethylethyl]-4-[2-[{methyl-2-propynylamino}methyl]-4thiazolyl]- (9CI) (CA INDEX NAME)

335242-68-7 CAPLUS Acetonitrile, [[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methylmethylamino]- [9CI] (CA INDEX NAME)

335242-69-8 CAPLUS Pentanenitrile, 5-[[[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methylmethylamino]- (9CI) (CA INDEX NAME)

 $\begin{array}{lll} 335242-70-1 & \text{CAPLUS} \\ \text{Hexanenitrile, } 6-[\{\{4-[3,5-\text{bis}\{1,1-\text{dimethylethyl}\}-4-\text{hydroxyphenyl}\}-2-\text{hydroxyphenyl}]-2-\text{hydroxyphenyl}] \\ \end{array}$

ANSWER 11 OF 18 CAPLUS COPYRIGHT 2006 ACS ON STN thiazolyl]methylamino]- (9CI) (CA INDEX NAME) (Continued)

RN 335242-71-2 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[{(2-hydroxyethyl)methylamino]meth
yl)-4-thiazolyl)- (9CI) (CA INDEX NAME)

RN 335242-72-3 CAPLUS
CN Phenol,
2,6-bis(1,1-dimethylethyl)-4-[2-[{methyl(phenylmethyl)amino]methyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Ph-CH}_2-\text{N-CH}_2 \\ \text{S} \end{array} \begin{array}{c} \text{t-Bu} \\ \text{OH} \\ \text{Bu-t} \end{array}$$

335242-75-6 CAPLUS
Phenol, 4-(2-(aminomethyl)-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI)(CA INDEX NAME)

335242-77-8 CAPLUS

RN 335242-77-8 CAPLUS
CN Phenol,
4-[2-[[(4-aminophenyl)methyl]methylamino]methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

ANSWER 11 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

●x HCl

335246-01-0 CAPLUS Phenol, 4-[2-[(methylamino)methyl]-4-thiazolyl]-, hydrochloride (9CI)

INDEX NAME)

●x HCl

335246-05-4 CAPLUS
Phenol, 4-[2-[{dimethylamino}methyl]-4-thiazolyl}-2,6-bis{1,1-dimethylethyl}-, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 335246-19-0 CAPLUS
CN Phenol,
2.6-bis(1.1-dimethylethyl)-4-{2-{(methylamino)methyl}-4-thiezolyl}, hydrochloride (9CI) (CA INDEX NAME)

L7 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN

$$\begin{array}{c} \text{He} \\ \text{Ho} \\ \text{L-Bu} \end{array} \xrightarrow{\text{N}} \begin{array}{c} \text{Me} \\ \text{S} \\ \text{CH}_2 - \text{N} - \text{CH}_2 \end{array} \xrightarrow{\text{N}} \begin{array}{c} \text{NH}_2 \\ \text{N} \\ \text{S} \end{array}$$

335242-79-0 CAPLUS
Phenol, 4-[2-[[[{4-aminophenyl}methyl]amino]methyl]-4-thiazolyl]-2,6-bis(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)

(Continued)

335242-81-4 CAPLUS
Butanenitrile, 4-[[(4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2-thiazolyl]methyl]methylamino}- (9CI) (CA INDEX NAME)

335242-82-5 CAPLUS
Phenol, 2,6-bis(1,1-dimethylethyl)-4-{2-{[[(3-nitrophenyl)methyl]amino]methyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

335245-99-3 CAPLUS
Phenol, 4-[2-[(methylamino)methyl]-4-thiazolyl]-2,6-bis(1-methylethyl)-,hydrochloride (9CI) (CA INDEX NAME)

ANSWER 11 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

●x HCl

335246-31-6 CAPLUS
Phenol, 4-[2-{[methylamino]methyl]-4-thiazolyl}-2,6-bis(1-methylethyl)-(9CI) (CA INDEX NAME)

335246-32-7 CAPLUS
Phenol, 4-[2-[(methylamino)methyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

335246-34-9 CAPLUS
Phenol, 4-{2-{(dimethylamino)methyl}-4-thiszolyl}-2,6-bis(1,1-dimethylethyl)-(9CI) (CA INDEX NAME)

218944-60-6F, 4-[3,5-Bis(1,1-dimethylethyl)-4-hydroxyphenyl]-N[(1,1-dimethylethoxy)carbonyl]-N-methyl-2-thiazolemethanamine
335247-51-3P, 4-[2-[(tert-Butoxycarbonyl)(methyl)amino]methyl}1,3-thiazol-4-yl]-2,6-diisopropylphenyl acetate 335247-52-48,
tert-Butyl [(4-(4-hydroxy-3,5-diisopropylphenyl)-1,3-thiazol-2yl]methyl](methyl)carbamate acetate 335247-53-5P, tert-Butyl
[(4-(4-hydroxyphenyl)-1,3-thiazol-2-yl]methyl](methyl)carbamate

ANSWER 11 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT L7

RI: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; prepn. of five-membered heterocycle derivs. as NAO inhibitors, lipid peroxidn. inhibitors, and sodium channel modulators) 218944-60-6 CAPLUS Carbamic acid, [[4-i3,5-bis[1,1-dimethylethyl]-4-hydroxyphenyl]-2-thiarolyl]methyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

335247-51-3 CAPLUS
Carbanic acid, [[4-[4-[acetyloxy]-3,5-bis[1-methylethyl]phenyl]-2thiazolyl]methylmethylm-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{t-BuO-C-N-CH}_2 \\ & \text{S} \\ & & \text{i-Pr} \end{array}$$

335247-52-4 CAPLUS
Carbamic acid, [[4-[4-hydroxy-3,5-bis(1-methylethyl]phenyl]-2thiazolyl]methyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

335247-53-5 CAPLUS Carbamic acid, [[4-(4-hydroxyphenyl)-2-thiazolyl]methyl]methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L7 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN ACCESSION NUMBER: 2000:900614 CAPLUS DOCUMENT NUMBER: 134:56958 DOCUMENT NUMBER: Preparation of amino acid derivatives as serine

protease inhibitors Liebeschuetz, John Walter; Lyons, Amanda Jane; INVENTOR(S): Murray,

Christopher William: Rimmer, Andrew David: Young, Stephen Clinton: Camp, Nicholas Paul: Jones, Stuart Donald: Morgan, Phillip John; Richards, Simon James; Wylie, William Alexander: Masters, John Joseph;

Wiley, Michael Robert Eli Lilly and Company, USA; Protherics Molecular Design Limited PCT Int. Appl., 261 pp. CODEN: PIXXD2 Patent

SOURCE:

DOCUMENT TYPE: LANGUAGE: English 13 LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT ASSIGNEE(S):

PA	rent	NO.			KIN								NO.					
w^	2000									WO 2000-GB2302						20000612		
20	2000	0769	71		A3 2001221					#O 2000-GB2302						20000613		
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								KG,										
								MW,										
								TM,										
			ZW,	J.,	JA,	55,	,	111,	ıĸ,	11,	10,	UA,	00,	03,	04,	V 14,	10,	
	RW:			KE.	LS.	MW.	MZ.	SD,	SI	82.	т2.	ug.	2W.	ΔТ.	BE.	CH.	CV	
								GR,										
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CA	2375		,					1221							2	aann	613	
ΑU	2000	0541	40		A5		2001	0102		AU 2	000-	5414	0		2	0000	613	
	1192				A2		2002	0403		EP 2	000-	9389	16		20000613			
EΡ	1192	132			B1		2005	0907										
	R:	AT,	BE,	CH,	DE.	DK,	ES,	FR,	GB,	GR.	IT.	LI.	LU.	NL.	SE.	MC.	PT.	
		ΙE,	SI,	LT,	LV,	FI,	RO											
JP	2003 3039	5023	14		T2		2003	0121		JP 2	001-	5038	31		2	0000	613	
ΑT	3039	8 8			E		2005	0915	1	AT 2	000-	9389	16		2	0000	613	
CA	2411	798			AA		2001	1220		CA 2	001-	2411	798		2	0010	612	
	2411							1220								0010	612	
WO	2001							1220								0010		
	W:							ΑZ,										
								DM,										
								15,										
								MG,										
							SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	
					ZA,													
	RW:							SD,										
								GR,								TR,	BF,	
		BJ,	CF,	CG,	CI,	CM,	GA,	GN,	G₩,	ML,	MR,	NE,	SN,	TD,	TG			
WO	2001																	
	W:							AZ,										
								DM,										
								15,										
		Tra,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	РΤ,	
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US 6784182
US 2003078438
        20040831
            US 2002-30189
                  20020204
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L7	ANSWER 12 OF 18	CAPLUS		06 ACS on STN	(Continued)
	US 6878725 US 2003109706	B2 A1	20050412 20030612	US 2002-301BB	20020204
	ZA 2002009153	A	20030612	ZA 2002-30188	20020204
	NO 2002005665	Â	20040213	NO 2002-5665	20021125
	HR 20020997	B1	20050228	HR 2002-997	20021212
	US 2003216403	Al	20031120	US 2003-296245	20030514
	HK 1054379	Al	20050324	HK 2003-106546	20030911
	US 2004142963	A1	20040722	US 2004-754923	20040112
	US 6936611	B2	20050830		
	US 2004176363	A1	20040909	US 2004-803157	20040318
	US 2004242656	A1	20041202	US 2004-876672	20040628
	US 2004259868	A1	20041223	US 2004-883715	20040706
	US 6900196	В2	20050531		
	US 2005032790	A1	20050210	US 2004-923010	20040823
PRIO	RITY APPLN. INFO.	:		GB 1999-13823	A 19990614
					•
				US 1999-142064P	P 19990702
				GB 1999~18741	A 19990809
				GB 1999-29553	A 19991214
				WO 2000-GB2302	W 20000613
				WO 2000-GB2302	w 20000013
				GB 2000-30303	A 20001213
				GD 2000-30303	A 20001213
				GB 2000-30304	A 20001213

				GB 2000-30305	A 20001213
				GB 2000-30306	A 20001213
				EP 2001-936686	A3 20010612
				WO 2001-GB2541	W 20010612
				WO 2001-GB2551	W 20010612
				WO 2001-GB2553	W 20010612
				WO 2001-GB2566	W 20010612
				WO 2001-G52366	# 20010612
				WO 2001-GB2572	W 20010612
				WO 2001-GB2372	# 20010012
				US 2001-926712	A3 20011206
				US 2002-30187	A1 20020204
				US 2002-30188	A3 20020204
				US 2002-30189	A3 20020204
OTHE	R SOURCE(S):	MARPA	T 134:56958		

R SOURCE(S): MARPAT 134:56958

Compds. R2-XX-Y-{(Cy)-L-Lp(D)n [R2 represents a 5- or 6-membered aromatic carbon ring optionally interrupted by a N, 0 or 5 ring atom, optionally substituted at the 3 and/or 4 position or forms a fused ring system at these positions, which is an optionally substituted 5 or 6 membered carbocyclic or heterocyclic ring or substituted at the position alpha to X-X; X is a C, N, 0 or S atom or a CO, CRIA, C(RIA)2 or NRIa group, where RIa represents H, OH, alkoxy, alkyl, aminoalkyl, hydroxyalkyl,

L7 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

ANSWER 12 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) alkoxyalkyl, alkoxycarbonyl, alkylaminocarbonyl, alkoxycarbonylamino, acyloxymathoxycarbonyl or alkylamino optionally substituted by OH, alkylamino, alkoxy, oxo, aryl or cycloalkyl; L is an org. linker group contg. 1 to 5 backbone atoms selected from C, N, O and S, or a branched alkyl or cyclic group; Y is a N atom or a CRIb group (Rib defined as for Ria); Cy is an (un)substituted, (un)satd., mono- or polycyclic, homo- or heterocyclic group; Lp is a lipophilic org. group; D is a hydrogen bond donor group; n = 0-2] were prepd. for use as serine protease inhibitors. Compds. of the invention were found to significantly elongate the partial thromboplastin time (prothrombin time). Thus, 1-(3-amino-2-naphthoyl-phenylglycinyl)-4,4'-bispiperidine was prepd. and shown to double the prothrombin time at a concn. of 26 µM.
313488-05-09
RL: BAC (Biological activity or effector, except adverse); BSU

BAC (Biological activity or effector, except adverse); BSU

RL: BAC (Biological activity or effector, enempt activity or effector, enempt activity or effector, enempt activity or effector, enempt activity, unclassified); SFN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREF (Preparation); USES (Uses) (preparation of amino acid derivs. as serine protease inhibitors) RN 313488-05-0 CAPLUS
CN | H-Indolm-6-carboxamide, 3-chloro-N-[(R)-[4-(4-methoxyphenyl)-2-thiazolyl]phenylmethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

313490-04-9P 313490-05-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
[preparation of amino acid derivs. as serine protease inhibitors)
313490-04-9 CAPLUS
Carbamic acid, {(R)-{4-(4-methoxyphenyl)-2-thiazolyl]phenylmethyl}-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

313490-05-0 CAPLUS 2-Thiazolemethanamine, 4-(4-methoxyphenyl)- α -phenyl-, (α R)-(9Cl) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 13 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN SSION NUMBER: 2000:900613 CAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER: 134:56957

TITLE:

Preparation of amino acid derivatives as serine protease inhibitors Liebeschuetz, John Walter; Lyons, Amanda Jane;

INVENTOR (S):

Christopher William: Rimmer, Andrew David; Young, Stephen Clinton: Camp, Nicholas Paul; Jones, Stuart Donald; Morgan, Phillip John: Richards, Simon James; Wylie, William Alexander: Lively, Sarah Elizabeth; Harrison, Martin James; Waszkowycz, Bohdan: Masters, John Joseph: Wiley, Michael John Eli Lilly and Company, USA; Protherics Molecular Design Limited
PCT Int. Appl., 350 pp.
CODEN: PIXXO2
Patent
English
13

APPLICATION NO.

PATENT ASSIGNEE(S):

SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.

DATE

US 1999-142064P P 19990702

> GB 1999-18741 A 19990809 GB 1999-29552 A 19991214 GB 1999-29553 A 19991214 WO 2000-GB2296 W 20000613

WO 2001-GB2566 W 20010612

OTHER SOURCE(S): MARPAT 134:56957

AB Compds. R2-X-X-Y(Cy)-L-Lp(D)n [R2 represents a 5- or 6-membered aromatic carbon ring optionally interrupted by a N, O or S ring atom, optionally substituted at the 3 and/or 4 position or forms a fused ring system at these positions, which is an optionally substituted 5 or 6 membered carbocyclic or heterocyclic ring; X is a C, N, O or S atom or a CO, CRla, C(Rla)2 or NRla group, where Rla represents H, OH, alkoxy, alkyl,

L7 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) aminoalkyl, hydroxyalkyl, alkoxyalkyl, alkoxycarbonyl, alkylaminocarbonyl, alkoxycarbonylamino, acyloxymethoxycarbonyl or alkylamino optionally substituted by OH, alkylamino, alkoxy, oxo, aryl or cycloalkyl; L is an org. linker group contg. 1 to 5 backbone atoms selected from C, N, O and S, or a branched alkyl or cyclic group; Y is a N atom or a CRIb group

(R1b) defined as for R1a); Cy is an (un)substituted, (un)satd., mono- or polycyclic, homo- or heterocyclic group; Lp is a lipophilic org. group is a hydrogen bond donor group; n = 0-2] were prepd. for use as serine protease inhibitors. Compds. of the invention were found to significantly elongate the partial thromboplastin time (prothrombin time). Thus, 1-(3-amino-2-naphthoyl-D-phenylglycinyl)-4,4'-bispiperidine was prepd. and

shown to double the prothrombin time at a concn. of 26 µM. 313488-05-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

logical study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of amino acid derivs. as serine protease inhibitors) 313488-05-0 CAPLUS H-Indole-6-carboxamide, 3-chloro-N-[(R)-[4-(4-methoxyphenyl)-2-thiazolyl]phenylmethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry

ΙT

313490-04-9P 313490-05-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
[preparation of amino acid derivs. as serine protease inhibitors)
313490-04-9 CAPLUS
Carbamic acid, [(R)-[4-(4-methoxyphenyl)-2-thiazolyl]phenylmethyl}-,
phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

CAPLUS 2-Thiazolemethanamine, 4-(4-methoxyphenyl)- α -phenyl-, (α R)-(9CI) (CA INDEX NAME)

L7 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2006 ACS ON STN ACCESSION NUMBER: 1999:27832 CAPLUS DOCUMENT NUMBER: 130:81398

Novel 2-(iminomethyl) aminophenyl derivatives as NO synthase inhibitors and traps for radical oxygen species TITLE:

INVENTOR(S):

species
Auvin, Serge; Harnett, Jeremiah; Bigg, Dennis;
Chabrier De Lassauniere, Pierre-Etienne
Societe De Consells de Recherches et D'Applications
Scientifiques (S.C.R.A.S, Fr.
PCT Int. Appl., 134 pp.
CODEN: PIXXO2 PATENT ASSIGNEE(S):

SOURCE:

DOCUMENT TYPE: Patent

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

9858934 A1 19981230 W0 1998-FR1250 19980615
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DZ, DK, EZ, ES, FI, GB, GE, GH, GM, GW, HU, ID, II, IS, JP, KE, KG, KP, KR, KZ, LC, IK, LR, IS, LT, LU, LV, MD, MG, MK, MN, MM, MX, NU, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW
RN: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BP, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG
2764889 B1 20000901
2764889 B1 20000901
2764889 B1 20000901
2764889 C1 20000901 PATENT NO. WO 9858934 CM, FR 2764889 FR 2764889 TW 422842 CA 2294809 AU 9882189 AU 737964 EP 991654 EP 991654 19990104 20010906 20000412 EP 1998-932205 19980615 20050615 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, FI, RO TR 1999-9903175 BR 1998-10197 NZ 1998-501656 JP 1999-503871 TR 9903175 T2 20000421 19980615 BR 9810197 20000808 19980615 NZ 501656 20011221 19980615 JP 2002507965 20020312 19980615 RU 2202543 C2 20030420 RU 2000-101328 19980615 AT 1998-932205 PT 1998-932205 ES 1998-932205 ZA 1998-5392 NO 1999-6208 AT 297935 20050715 19980615 PT 991654 ES 2244068 20051031 19980615 20051201 19980615 ZA 9805392 NO 9906208 NO 9906208 NO 315321 MX 9911971 HX 1030218 US 6630461 US 2002045753 US 659903 US 2002042511 US 6586454 US 2003078420 US 609088 US 2005043397 US 2005187272 9805392 19990120 19980619 20000215 19991215 20030818 20000430 MX 1999-11971 19991217 A A1 B2 A1 B2 A1 B2 A1 B2 20051028 20020117 20031007 HK 2001-101230 US 2001-882264 20010615 20020418 US 2001-945782 20010904 20030729 20020411 20030701 20030424 US 2001-953682 20010917 US 2002-191950 20020709 20041026 20050224 US 2004-898916 US 2005-105291 20040726 20050413

L7 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) Absolute stereochemistry,

L7 ANSWER 14 OF 18 CAPLUS	COPYRIGHT 2006 ACS on STN	(Continued)
PRIORITY APPLN. INFO.:	FR 1997-7701	A 19970620
	FR 1997-3528	A 19970324
	WO 1998-FR288	W 19980216
	WO 1998-FR1250	W 19980615
	US 1999-381749	A2 19990922
	US 1999-456205	A3 19991207
	US 2001-882264	A3 20010615
	US 2002-191950	A3 20020709
	US 2004-898916	A3 20040726

OTHER SOURCE(S): MARPAT 130:81398

Amidines AXHetYC6H4N:CBNH2 [A = H, (un)substituted HOC6H4, 6-hydroxy-2,5,7,8-tetramethylchroman-2-yl; B = (un)substituted alkyl, Ph, pyridyl, thienyl, furyl, pyrrolyl, thiacolyl; X = (un)substituted CONHX1, NHCOX1, CH:, CO, bond; X1 = (CH2)n; n = 0-6; Y = Y1, CONHY1, NHCOY1,

COY1, Y1CO, (un) substituted NHY1, Y1NH, Y1CH2NHCO, OY1, SY1, Y1S, Y1OY1,

YINHYI Y1 = (CH2)n; Het = (un)substituted heterocyclic] were prepared for use as NO synthetase inhibitors and reactive oxygen species traps. Thus, 4-PC6H4NO2

was treated with imidazole and the 1-p-nitrophenylimidazole reduced to

amine and treated with the thiophene fragment to give the amidine I. I had an NO synthetase-inhibiting IC50 < 3.5 μ M. 21894-60-69 218944-61-7P

RE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of novel 2-(iminomethyl)aminophenyl derivs. as NO

nase
inhibitors and traps for radical oxygen species)
218944-60-6 CAPLUS
Carbamic acid, [[4-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-2thiazolyl|methyl|methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

ANSWER 14 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN

218944-61-7 CAPLUS

RN 218944-61-7 CAPLUS
CN Phenol,
2,6-bis[l,1-ddimethylethyl)-4-[2-[{methylamino}methyl]-4-thiazolyl]{9CI} (CA INDEX NAME)

REFERENCE COUNT: THIS

THERE ARE 25 CITED REFERENCES AVAILABLE FOR 25

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 15 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN

L7 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:671691 CAPLUS
DOCUMENT NUMBER: 119:271691
Synthesis and antitrypanoscmal evaluation of some thiazole-containing amino acids and peptides
AUTHOR(S): Van Bogaert, I.; Haemers, A.; Bollaert, W.; Van Meirvenne, N.; Brun, R.; Smith, K.; Fairlamb, A. H.
CORPORATE SOURCE: Dep. Pharm. Chem., Univ. Antwerp, Antwerp, B-2610, Belg.
SOURCE: European Journal of Medicinal Chemistry (1993),

387-97 CODEN: EJMCA5; ISSN: 0223-5234 Journal English CASREACT 119:271691

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

Several amino acids and peptides containing thiszole and thiszolidine

residues

were prepared Thiazole-containing amino acids and peptides I (R1 = H, R2 = H, C02H, Ph; R1 = C02H, CH2C02H, Me, Ph, 0-MeOC6H4, m-MeOC6H4, p-MeOC6H4, p-C1C6H4, m-O2NC6H4, p-O2NC6H4, CO-Gly-OH, R2 = H), II, III and IV (R1 = OEt, Gly-OEt) were prepared These compds. were tested in vivo and in

as possible antitrypanosomal agents. Some derivs, showed a slight activity. As they are structurally related to glutathione, their inhibitory properties towards glutathion/lapermidine synthetase, trypanothione synthetase and trypanothione reductase were determined No inhibitory activity was found.

150715-82-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
150715-82-5 CAPLUS
2-Thiazolebutanoic acid, α-amino-4-(4-methoxyphenyl)- (9CI) (CA INDEX NAME) vitro

IT

L7 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:583277 CAPLUS
DOCUMENT NUMBER: 115:183277 CAPLUS
ITITLE: buty1-4-hydroxyphenyl)thiazoles
INVENTOR(S): Thorwart, Werner; Schleyerbach, Rudolf; Bartlett, Robert; Weithmann, Klaus Ulrich
HOGE-THE ACSIGNEE(S): Germany
DOCUMENT TYPE: CODE: EPXXDW
DOCUMENT TYPE: CODE: EPXXDW
DOCUMENT TYPE: German
FAMILU ACC. NUM. COUNT: 1
FAMILU ACC. NUM. COUNT: 1

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 432740	A2	19910619	EP 1990-123853	19901211
EP 432740	A3	19920102		
EP 432740	B1	19950308		
R: AT, BE, CH,			GR, IT, LI, LU, NL,	SE
DE 3941438	A1	19910620	DE 1989-3941438	19891215
FI 9006141	A	19910616	FI 1990-6141	19901213
HU 58306	A2	19920228	HU 1990-8258	19901213
HU 209584	В	19940829		
US 5137897	Ā	19920811	US 1990-626784	19901213
RU 2017739	C1	19940815	RU 1990-4894048	19901213
RU 2021264	C1	19941015	RU 1990-4894274	19901213
CA 2032282	AA	19910616	CA 1990-2032282	19901214
NO 9005411	A.	19910617	NO 1990-5411	19901214
AU 9068024	A1	19910620	AU 1990-68024	19901214
AU 630261	B2	19921022	AG 1550 00024	1330111
ZA 9010067	A	19910925	ZA 1990-10067	19901214
JP 05017459	Ã2	19930126	JP 1990-419334	19901214
PRIORITY APPLN. INFO.:	~-	13330120	DE 1989-3941438 A	
THEO.			DD 1303 3311430 A	

OTHER SOURCE(S): MARPAT 115:183277

AB Title compds. I [X = alkylene, alkenylene, optionally containing heteroatoms;

R = tetrazolyl, cyano, CO2H, esterified CO2H, (un) substituted CONH2; XR = (un) substituted 2-oxo-3-pyrrolidinylidenemethyl; R1 = CMe3, Me; R2 = H, Me] were prepared by various routes. Thus, 4,3,5-Ho(Me3C;2C6H2AC was treated with Et02CSCH2CH2CONH2; followed by ester hydrolysis to give I (X = CH2CH2, R = CO2H, R1 = CMe3, R2 = H) which had a ED50 of 0.9 mg/kg orally in the adjuvant arthritis test.

IT 136203-18-49

R1: SPN (Synthetic preparation); PREP (Preparation) (preparation and antiarthritic activity of)

(Continued)

ANSWER 16 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Contin 136203-18-4 CAPLUS Phenol, -bis(1,1-dimethylethyl)-4-[2-[2-(1H-tetrazol-5-ylamino)ethyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

ANSWER 17 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) ANSWER I. OF 18 CAPLUS COPTRIGHT 2006 ACS on STM (Continued) was hydrolyzed with concd. Hcl under reflux to give 67% 2-(aminomethyl)-4-(indol-3-yl)thizzole Hcl [II]. A mixt. of II, 2-methyl-2-thiopseudoures sulfate, and AcONa in isopropanol was heated to reflux overnight to give 83% thiazole salt III. Addnl. 25 I were prepd. 132233-98-69 IT

132233-98-69
RE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as serotoninergic S3 antagonist)
132253-98-6 CAPLUS
Guanidine, [{4-(4-methoxyphenyl)-2-thiazolyl]methyl]- (9CI) (CA INDEX

L7 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN ACCESSION NUMBER: 1991:101982 CAPLUS

DOCUMENT NUMBER: 114:101982

TITLE:

114:101982
Preparation of heterocyclic guanidines as SHT3
antagonists
Nagel, Arthur A.; Rizzi, James P.; Rosen, Terry J.
Pfizer Inc., USA
U.S., 7 pp.
CODEN: USXXXM INVENTOR(S):

PATENT ASSIGNEE (S): SOURCE: DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4963689		19901016	US 1989-349189	19890509
EP 397364	Al	19901114	EP 1990-304684	19900430
EP 397364	Bi	19930728	2	
R: AT, BE, CH			B, GR, IT, LI, LU, NL,	SE
AT 92062	E E	19930815	AT 1990-304684	19900430
ES 2058795	T3	19941101	ES 1990-304684	19900430
IL 94254	Al	19940530	IL 1990-94254	19900502
CA 2016182	AA	19901109	CA 1990-2016182	19900507
CA 2016182	č	19960312	u. 1550 2010112	
AU 9054767	Ã1	19901115	AU 1990-54767	19900507
AU 615385	B2	19910926		••••
NO 9002029	A	19901112	NO 1990-2029	19900508
ZA 9003478	Ä	19911224	ZA 1990-3478	19900508
JP 03011070	A2	19910118	JP 1990-119635	19900509
JP 06035454	84	19940511		
HU 58063	A2	19920128	HU 1990-2976	19900509
PRIORITY APPLN. INFO.:		13324120	US 1989-349189	A 19890509

OTHER SOURCE(S):

CASREACT 114:101982; MARPAT 114:101982

GHC1 III

Ar-Het-CH2NRIC(:NR2)NHR3 (I; Ar = naphthyl, indol-3-yl, 2-methylindol-3-yl, 1-methylindol-3-yl, 1-benzylindol-3-ylphenyl, mono-or disubstituted Ph; Het = 4-thiazol-2-yl, 3-isoxazol-5-yl, 2-thien-5-yl, 2-fur-5-yl; R1 = H, Me; R2, R3 = H, hydroxyalkyl, alkyl, cycloalkyl,

or R2R3 = C2,3 alkylene), useful for treatment of nausea, anxiety, pain, schizophrenia, and gastrointestinal disorders (no data), are prepared

a solution of 3-(chloroacetyl)indole and AcNHCH2C(S)NH2 in EtOH was refluxed overnight to give 51% 2-(N-acetylaminomethyl)-4-(indol-3-yl)thiazole which

L7 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1961:137431 CAPLUS
DOCUMENT NUMBER: 55:137431
CORPICIONAL REFERENCE NO: 55:25917g-1,25918a-e
COMPLEX FORMING COMPOUNDS of the thiazole series
AUTHOR(S): Complex-forming compounds of the thiazole series
AUTHOR(S): Univ. Basel, Switz.
SOURCE: Helvetica Chimica Acta (1960), 43, 659-64
CODEN: HCACAV; ISSN: 0018-019X
JOURNAL LANGUAGE: German
OTHER SOURCE(S): CASREACT 55:137431

OTHER SOURCE(S):

UAGE: German

R SOURCE(s): CASREACT 55:137431

Compds. with potential metal-chelating properties having 2 or 4 basic groups of partly aromatic, partly aliphatic character were synthesized. (NHZCH2)2 (44 g. in 94 ml. H20) was treated dropwise with stirring and cooling with 50 g. HCN and with 1.14 g. Ca(CN)2 in 12.5 ml. H20, and the mixture stirred an addnl. 0.5 hr., saturated with NaCl, and extracted

mixture stirred en addnl. 0.5 hr., saturated with NaCl, and extracted ether 5 days in a Kutscher-Streudel apparatus to give 57.5% ethylenediamine-N,N'-diacatonitrile (1). I was acetylated to the N,N'-diacetyl derivative, m. 169-71 (MeOR), which (1 g. in 100 ml. hot absolute alc.) was treated with 2-3 ml. Et3N and with H2S (3 hrs.) to give 61.5% N,N'-diacetylethylenediamine-N,N'dithioacetamide (II), decomposing 214-18°. II (900 mg.) was refluxed 2 hrs. with 960 mg. p-ClC6H4COCH2Br in 50 ml. EtOH containing 2-3 drops CSH3N to give 65% N,N'-diacetyl-N,N'-bis [4-(p-chlorophenyl)-2-thiazolylmethyl] ethylenediamine (III), m. 206-8°. Similariy prepared, from the appropriate phenacyl bromide, were the p-bromophenyl (IV), m. 214-16°, p-tolyl (V), m. 170-2°, and p-methoxyphenyl analogs (VI), m. 180-3°. III (200 mg.) heated 4 hrs. at 100° with 5 ml. concentrated HCl and 5 ml. EtOH and the product filtered off at 0° and washed with absolute alc. gave 92% N,N'-bis [4-(p-chlorophenyl)-2-thiazolylmethyl] ethylenediamine-2RCl, decomposing 248-55°, heated 3 min. at 80° with 20% NaOAc to give the free base. Similarly, IV, V, and VI were deacetylated to give dihydrochlorides m. 258-64° (free base m. 145-7°), 241-7°, and 252-6° (free base m. 258-64° (free base m. 145-7°), 241-7°, and 252-6° (free base m. 258-64° (free base m. 16-17°), resp. Absolute alc. (25 ml.) and 2 ml. Et3N saturated with H2S at 0°, treated with 10°, piperazine-N,N'-diacetonitrile, and kept in an autoclave 12 hrs. at 70-5° gave 71% piperazine-N,N'-dithlocatemide (VII). VII (232 g.) refluxed 3 hrs. with 5.88 g. p-Brc6H4COCH2Br in 100 ml. absolute alc. with 2-3 drops C5H5N gave 97% N, N'-bis [4-(p-bromophenyl)-2-thiazolylmethyl]piperazine dihydrobromide 17 2HBr), decomposing 276-86° (EtOH), of which 1 g. shaken with 1:1 NH4OH with

(VIII

2 Public 1- Descriptions 276-86° (EtON), of which 1 g. shaken with 1:1 NH4OH (and the product washed) gave VIII, m. 252-8° (CSH6). Similarly, VII with p-MeoCSH4COHZBY gave the p-methoxyphenyl analog, m. 214-17°. (Piperidino) thioactehaide (IX) (5 g.) refluxed 14 hrs. with 5.8 g. AcCH2Cl in 50 ml. absolute alc., the mixture cooled to 0°, filtered, and eveporated in vacuo c50°, the residue taken up in 20 ml. 2N HCl, the solution shaken with C 0.5 hr. and extracted with 2 + 50 ml. ether, the extract discarded, and the solution made basic at 0° with 2N NAOH and extracted with ether 48 hrs. in a Kutscher-Streudel apparatus 19.48

19.48
2-piperidinomethylthiazole; picrate m. 140-2°. IX treated with PsPrG6H4-COCHZBr gave a hydrobromide that on warming with 2N NaOH gave 2-piperidinomethyl-4-(p-bromophenyl)thiazole, m. 110-11° (1:10 H20-alc.). The p-methoxyphenyl analog, m. 88-9°, was similarly prepared N-Acetylsarcosine-thioamide was condensed with the appropriate phenacyl bromide to form 2-(N-acetylmethylaminomethyl)-4-(p-bromophenyl)thiazole, m. 98-101° (MeOH), or the p-methoxyphenyl (m. 114-16°) and p-chlorophenyl analog (not isolated). Each was

ANSWER 18 OF 18 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) deacetylated to give 2-methylaminomethyl-4-(p-bromophenyl)thiazole, m. 82-3* (1:1 aq. MeOH); HCl salt m. 226-8*, and the p-methoxyphenyl (X) (m. 40-1*; HCl salt m. 207-11*) and p-chlorophenyl analog (XI) (m. 70-2*; HCl salt m. 222-6*). The 1:1 Cu++ complexes of X and XI showed an extinction coeff. little different from that of CuS04.

100134-70-1, Thiazole, 4-(p-methoxyphenyl)-2-(methylaminomethyl)- (and derivs.)
100134-70-1 CAPLUS
Thiazole, 4-(p-methoxyphenyl)-2-(methylaminomethyl)- (6CI) (CA INDEX NAME)

103155-61-9, Acetamide, N-[[4-(p-methoxyphenyl)-2-thiazolyl]methyl]-N-methyl- 104339-29-9, Acetamide, N,N'-ethylenebis[N-[[4-(p-methoxyphenyl)-2-thiazolyl]methyl]-(preparation of) 103155-61-9 CAPLUS Acetamide, N-[[4-(p-methoxyphenyl)-2-thiazolyl]methyl]-N-methyl- (6CI) (CA INDEX NAME)

104339-29-9 CAPLUS
Acetamide, N,N'-ethylenebis[N-{[4-{p-methoxyphenyl}-2-thiazolyl]methyl]-(6CI) (CA INDEX NAME)

=> fil reg SINCE FILE COST IN U.S. DOLLARS TOTAL ENTRY SESSION FULL ESTIMATED COST 92.44 291.41 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -13.50 -13.50

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STRUCTURE FILE UPDATES: 23 MAY 2006 HIGHEST RN 885357-09-5 DICTIONARY FILE UPDATES: 23 MAY 2006 HIGHEST RN 885357-09-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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* The CA roles and document type information have been removed from * the IDE default display format and the ED field has been added, * effective March 20, 2005. A new display format, IDERL, is now * available and contains the CA role and document type information. * *

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

Uploading C:\Program Files\Stnexp\Queries\QUERIES\106810021.str

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chain nodes :
6 7 8 16 17 18 19 20 23 24 25 27 28 29 32
ring nodes :
1 2 3 4 5 10 11 12 13 14 15
chain bonds :
2-6 3-15 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28 8-29 10-20 11-19 12-16
13-17 14-18
ring bonds :
1-2 1-5 2-3 3-4 4-5 10-11 10-15 11-12 12-13 13-14
                                                   14-15
exact/norm bonds :
1-2 1-5 2-3 2-6 3-4 3-15 4-5 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28
8-29 10-20 11-19 12-16 13-17 14-18
normalized bonds :
10-11 10-15 11-12 12-13 13-14 14-15
isolated ring systems :
containing 1 : 10 :
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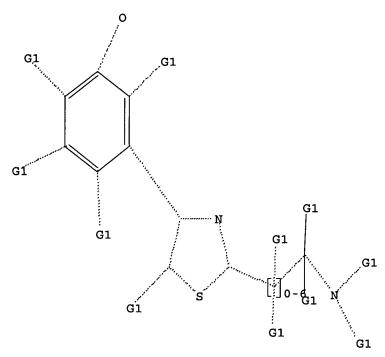
G1:C,H

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 23:CLASS 24:CLASS 25:CLASS 27:CLASS 28:CLASS 29:CLASS 32:CLASS

L8 STRUCTURE UPLOADED

=> d L8 HAS NO ANSWERS L8 STR



G1 C,H

Structure attributes must be viewed using STN Express query preparation.

2 ANSWERS

=> s 18

SAMPLE SEARCH INITIATED 08:49:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 30 TO ITERATE

100.0% PROCESSED 30 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 272 TO 928

PROJECTED ANSWERS: 2 TO 124

L9 2 SEA SSS SAM L8

=> s 18 full

FULL SEARCH INITIATED 08:49:16 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 816 TO ITERATE

100.0% PROCESSED 816 ITERATIONS 20 ANSWERS

SEARCH TIME: 00.00.01

L10 20 SEA SSS FUL L8

=> s 110 and caplus/lc 50652292 CAPLUS/LC

L11 1 L10 AND CAPLUS/LC

=> s 110 not 111 L12 19 L10 NOT L11

=> d 112 1-19

L12 ANSWER 1 OF 19 REGISTRY COPYRIGHT 2006 ACS on STN

RN 761403-31-0 REGISTRY
ED Entered STN: 13 Oct 2004
Acctamide, 2,2-trifluoro-N-[2-[4-(3-hydroxyphenyl)-2-thiazolyl]ethyl](9CI) (CA INDEX NAME)
S 3D CONCORD
MF C13 H11 F3 N2 O2 S
Chemical Library
Supplier: Timfec, Inc.
LC STN Files: CHEMCATS

$$\underset{\texttt{F}_3\texttt{C}-\texttt{C}-\texttt{NH}-\texttt{CH}_2-\texttt{CH}_2-\texttt{NH}-\texttt{OH}}{\overset{\bullet}{\bigcap}}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

MeNH-CH2

L12 ANSWER 5 OF 19 REGISTRY COPYRIGHT 2006 ACS on STN
RN 643725-29-5 REGISTRY
CD Entered STN: 30 Jan 2004
CN 2-Thiazolemethanamine, 4-[3-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
HZ C17 H16 N2 O S
SR Chemical Catalog
Supplier: ACB Blocks Ltd
LC STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 ANSWER 7 OF 19 REGISTRY COPYRIGHT 2006 ACS on STN

RN 643723-49-3 REGISTRY
ED Entered STN: 30 Jan 2004
CN 2-Thiezolemethanamine, 4-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)
SS 3D CONCORD
FC C11 H12 N2 O S
SR Chemical Catalog
Supplier: ACB Blocks Ltd
LC STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 ANSWER 6 OF 19 REGISTRY COPYRIGHT 2006 ACS on STN

RN 643725-28-4 REGISTRY
ED Entered STN: 30 Jan 2004
C 2-Thiazolemethanamine, 4-(3-ethoxyphenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
FC 12 H14 N2 O S
Chemical Catalog
Supplier: ACB Blocks Ltd
LC STN Files: CHENCATS

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT **

L12 ANSWER 8 OF 19 REGISTRY COPYRIGHT 2006 ACS on STN
RN 643023-86-3 REGISTRY
ED Entered STN: 29 Jan 2004
C 2-Thiazolemethanamine, N,α-dimethyl-4-[3-(phenylmethoxy)phenyl](9CI) (CA INDEX NAME)
S 3D CONCORD
MF C19 H20 N2 O S
SR Chemical Catalog
Supplier: ACB Blocks Ltd
LC STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

`0— СH2— Ph

L12 ANSWER 9 OF 19 REGISTRY COPYRIGHT 2006 ACS on STN
RN 643023-95-2 REGISTRY
ED Entered STN: 29 Jan 2004
N 2-Thia colemethanamine, 4-(3-ethoxyphenyl)-N,α-dimethyl- (9CI) (CA INDEX NAME)
BJ CONCORD
FS 3D CONCORD
FC 14 HI8 N2 O S
SR Chemical Catalog
Supplier: ACB Blocks Ltd
LC STN Files: CHEMCATS

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT **

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 ANSWER 13 OF 19 REGISTRY COPYRIGHT 2006 ACS on STN
RN 642929-32-0 REGISTRY
ED Entered STN: 29 Jan 2004
CA 2-Thiezolemethanamine, 4-(3-methoxyphenyl)-\alpha-methyl- (9CI) (CA
INDEX NAME)
FS 3D CONCORD
MF C12 H14 N2 O S
SR Chemical Catalog
Supplier: ACB Blocks Ltd
LC STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 ANSWER 15 OF 19 REGISTRY COPYRIGHT 2006 ACS on STN
RN 642928-91-4 REGISTRY
ED Entered STN: 29 Jan 2004
CN 2-Thiazoleethanamine, 4-(3-ethoxyphenyl)-N-methyl- (9CI) (CA INDEX NAME)
F3 3D CONCORD
MF C14 H18 N2 O S
SR Chemical Catalog
Supplier: ACB Blocks Ltd
LC STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 ANSWER 14 OF 19 REGISTRY COPYRIGHT 2006 ACS ON STN
RN 642928-93-6 REGISTRY
ED Entered STN: 29 Jan 2004
C 2-Thiazoleethanamine, N-methyl-4-{3-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)
S 3D CONCORD
MF C19 H20 N2 O S
SR Chemical Catalog
Supplier: ACB Blocks Ltd
LC STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

MeNH-CH2-CH2

L12 ANSWER 17 OF 19 REGISTRY COPYRIGHT 2006 ACS on STN
RN 642080-19-1 REGISTRY
ED Entered STN: 27 Jan 2004
C 2-Thiazoleethanamine, 4-[3-[phenylmethoxy]phenyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
FC 18 H18 N2 O S
Chemical Catalog
Supplier: ACB Blocks Ltd
LC STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 ANSWER 18 OF 19 REGISTRY COPYRIGHT 2006 ACS ON STN
RN 642080-18-0 REGISTRY
ED Entered STN: 27 Jan 2004
C 2-Thiazoleethanemine, 4-(3-ethoxyphenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
FC 13 H16 N2 O S
Chemical Catalog
Supplier: ACB Blocks Ltd
LC STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L12 ANSWER 19 OF 19 REGISTRY COPYRIGHT 2006 ACS on STN
RN 642078-08-8 REGISTRY
ED Entered STN: 27 Jan 2004
C 2-Thiazoleethanamine, 4-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
FC C12 H14 N2 O S
Chemical Catalog
Supplier: ACB Blocks Ltd
LC STN Files: CHEMCATS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

=> fil caplus COST IN U.S. DOLLARS SINCE FILE TOTAL SESSION ENTRY FULL ESTIMATED COST 207.80 499.21 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -13.50

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FILE COVERS 1907 - 24 May 2006 VOL 144 ISS 22 FILE LAST UPDATED: 23 May 2006 (20060523/ED)

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=> s l11 L13 1 L11

=> d ibib abs hitstr

L13 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:671691 CAPLUS
DOCUMENT NUMBER: 119:271691 Synthesis and antitrypanosomal evaluation of some thiazole-containing amino acids and peptides
AUTHOR(S): Van Bogaert, I.; Haemers, A.; Boilaert, W.; Van Meirvenne, N.; Brun, R.; Smith, K.; Fairlamb, A. H.
CORPORATE SOURCE: Dep. Pharm. Chem., Univ. Antwerp, Antwerp, B-2610, Belg.
SOURCE: European Journal of Medicinal Chemistry (1993),

387-97 CODEN: EJMCA5; ISSN: 0223-5234 Journal English CASREACT 119:271691

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

AB Several amino acids and peptides containing thiazole and thiazolidine residues were prepared Thiazole-containing amino acids and peptides I (R1 = H, R2 = H, CO2H, Ph; R1 = CO2H, CH2CO2H, Me, Ph, c-MeoC6H4, m-MeoC6H4, p-MeoC6H4, p-C1C6H4, m-O2NC6H4, p-O2NC6H4, CO-G1y-OH, R2 = H), II, III and IV (R1 = OEt, Gly-OEt) were prepared These compds. were tested in vivo and in vitro

OEC, Gly-OEC) were prepared These compds. were tested in vivo and in Vitro

as possible antitrypanosomal agents. Some derivs. showed a slight activity. As they are structurally related to glutathione, their inhibitory properties towards glutathionylspermidine synthetase, trypanothione synthetase and trypanothione reductase were determined No inhibitory activity was found.

IT 150715-01-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 150715-01-4 CAPLUS

CN 2-Thiazolebutanoic acid, α-amino-4-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)

L13 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

=> fil reg COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

504.78 5.57

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE

-0.75 -14.25

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STRUCTURE FILE UPDATES: 23 MAY 2006 HIGHEST RN 885357-09-5 DICTIONARY FILE UPDATES: 23 MAY 2006 HIGHEST RN 885357-09-5

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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* The CA roles and document type information have been removed from * * the IDE default display format and the ED field has been added, * effective March 20, 2005. A new display format, IDERL, is now st available and contains the CA role and document type information. st

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

Uploading C:\Program Files\Stnexp\Queries\QUERIES\106810021.str

chain nodes : 6 7 8 16 17 18 19 20 23 24 25 27 28 29 32 ring nodes : 1 2 3 4 5 10 11 12 13 14 15 chain bonds : 2-6 3-15 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28 8-29 10-20 11-19 12-16 13-17 14-18 ring bonds : 1-2 1-5 2-3 3-4 4-5 10-11 10-15 11-12 12-13 13-14 14-15 exact/norm bonds : 1-2 1-5 2-3 2-6 3-4 3-15 4-5 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28 8-29 10-20 11-19 12-16 13-17 14-18 normalized bonds : 10-11 10-15 11-12 12-13 13-14 14-15 isolated ring systems : containing 1 : 10 :

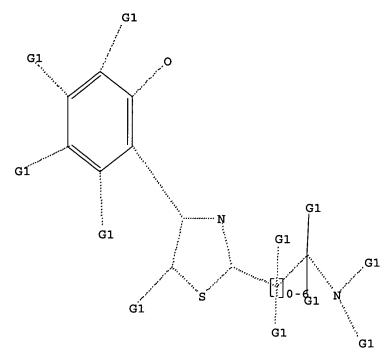
G1:C,H

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 23:CLASS 24:CLASS 25:CLASS 27:CLASS 28:CLASS 29:CLASS 32:CLASS

L14 STRUCTURE UPLOADED

=> d L14 HAS NO ANSWERS L14 STR



G1 C,H

Structure attributes must be viewed using STN Express query preparation.

=> s 114

SAMPLE SEARCH INITIATED 08:50:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 86 TO ITERATE

100.0% PROCESSED 86 ITERATIONS 4 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 1164 TO 2276

PROJECTED ANSWERS: 4 TO 200

L15 4 SEA SSS SAM L14

=> s l14 full

FULL SEARCH INITIATED 08:50:59 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1535 TO ITERATE

100.0% PROCESSED 1535 ITERATIONS 189 ANSWERS

SEARCH TIME: 00.00.01

L16 189 SEA SSS FUL L14

=> s l16 and caplus/lc 50652292 CAPLUS/LC

L17 9 L16 AND CAPLUS/LC

=> s 116 not 117 L18 180 L16 NOT L17

=> d l18 160

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

```
L18 ANSMER 180 OF 180 REGISTRY COPYRIGHT 2006 ACS ON STN
RN 642078-06-6 REGISTRY
ED Entered STN: 27 Jan 2004
C 2-Thiazolecthanemine, 4-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
FC 112 H14 N2 O S
Chemical Catalog
Supplier: ACB Blocks Ltd
LC STN Files: CHEMCATS
```

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

=> fil caplus
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST

176.38 681.16

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE

0.00 -14.25

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FILE COVERS 1907 - 24 May 2006 VOL 144 ISS 22 FILE LAST UPDATED: 23 May 2006 (20060523/ED)

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=> s 117

L19 5 L17

=> d ibib abs hitstr 1-5

L19 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:316737 CAPLUS
DOCUMENT NUMBER: 144:370549
TITLE: Heterocycle-amine ligands, compositions, complexes, and catalysts, and methods of making and using the

and catalysts, and methods of maxing and using the same Diamond, Gary; Lapointe, Anne M.; Leclerc, Margarete K.; Longmire, James; Nava-Salgado, Victor; Shoemaker, James A. W.; Sun, Pu Symyx Technologies, Inc., USA PCT Int. Appl., 219 pp. CODEN: PIXXD2 Patent English INVENTOR (S):

PATENT ASSIGNEE (S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

WO 2006036748 A2 20060406 WO 2005-U334009 20050921
W: AR, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CH, CO, CC, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, NA, NG, NI, NO, NZ, CM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SI, SM, SY, TJ, TM, TM, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LIT, LU, LV, MC, NL, PI, PT, RO, SE, SI, SK, TR, BF, BJ, CP, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, NM, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
US 2006094867 A1 200609504 US 2005-233227 20050921
PRIORITY APPIN. INFO:

Ligands, compns., and metal-ligand complexes that incorporate heterocycle-amine compds. are disclosed that are useful in the catalysis of transformations such as the polymerization of monomers into polymers. AB

catalysts have high performance characteristics, including higher commonmer incorporation into ethylene/olefin copolymers, where such olefins are for example, 1-octone, propylene or styrene. The catalysts also polymerize propylene to form isotactic polypropylene. 881998-65-68 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); IT

RACT

Reactant or reagent)
(ligand; manufacture of complexes containing heterocycle-amine
ligands for use
in olefin polymerization)
RN 881998-65-8 CAPIUS
CN Pheol, 2-[2-[[[2,6-bis(1-methylethyl)phenyl]amino]phenylmethyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

L19 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:908905 CAPLUS
DOCUMENT NUMBER: 142:68509
TITLE: A 3D Similarity Method for Scaffold Hopping from
Known

AUTHOR(S): CORPORATE SOURCE:

Drugs or Natural Ligands to New Chemotypes
Jenkins, Jeremy L.; Glick, Meir; Davies, John W.
Lead Discovery Center, Novartis Institutes for
BioMedical Research Inc., Cambridge, MA, 02139, USA
JOURNAL of Medicinal Chemistry (2004), 47(25),
6144-615
CODEN: JMCMAR; ISSN: 0022-2623
American Chemical Society
Journal

SOURCE .

PUBLISHER: DOCUMENT TYPE:

MENT TYPE: JOURNAL DAGE: English English Searching is to find compds. with similar A primary goal of 3D similarity searching is to find compds. with similar bloactivity to a reference ligand but with different chemotypes, i.e., "scaffold hopping". However, an adequate description of chemical

tures
in 3D conformational space is difficult due to the high-dimensionality of
the problem. The authors present an automated method that simplifies
flexible 3D chemical descriptions in which clustering techniques
traditionally used in data mining are exploited to create "fuzzy" mol.
representations called FEPOPS (feature point pharmacophores). The
representations can be used for flexible 3D similarity searching given

one

or more active compds. without a priori knowledge of bioactive conformations or pharmacophores. The authors demonstrate that similarity searching with FEPOPS significantly enriches for actives taken from inhouse high-throughput screening datasets and from MDDR activity classes COX-2, 5-HT3A, and HIV-RT, while also scaffold or ring-system hopping to new chemical frameworks. Further, inhibitors of target proteins (dopamine 2 and retinoic acid receptor) are recalled by FEPOPS by scaffold hopping from their associated endogenous ligands (dopamine and retinoic acid). Importantly, the method excels in comparison to commonly used 2D similarity methods (DAYLIGHT, NACCS, Pipeline Pilot fingerprints) and a com. 3D method (Pharmacophore Distance Triplets) at finding novel scaffold classes given a single guery mol

classes given a single query mol. 132254-03-6

132254-03-6
RL: PAC (Pharmacological activity); BIOL (Biological study)
(30 similarity method for scaffold hopping from known drugs or natural ligands to new chemotypes)
132254-03-6 CAPLUS
Guanidine, {{4-(2-methoxyphenyl)-2-thiazolyl}methyl}- (9CI) (CA INDEX NAME)

REFERENCE COUNT: THIS

73 THERE ARE 73 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L19 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

881998-64-7 881999-94-6
RI: RCT (Reactant); RACT (Reactant or reagent)
(manufacture of complexes containing heterocycle-amine ligands for in olefin
polymerization)
881998-64-7 CAPUS
2-Thiazolemethanamine, N-[2,6-bis(1-methylethyl)phenyl]-4-[2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]phenyl]-a-phenyl- (9CI) (CA INDEX NAME)

881999-94-6 CAPLUS
Phenol, 2-[2-[[[2,6-bis(1-methylethyl)phenyl]amino](2,4,6trimethylphenyl]methyl]-4-thlazolyl]- (SCI) (CA INDEX NAME)

L19 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

L19 ANSWER 3 OF 5
ACCESSION NUMBER:
DOCUMENT NUMBER:
INVENTOR(S):

PATENT ASSIGNEE(S):
SOURCE:

DOCUMENT TYPE:
LANGUAGE:

DOCUMENT TYPE:
LANGUAGE:

LANGUAGE:

CAPLUS COPYRIGHT 2006 ACS on STN
2004:878382 CAPLUS
141:350161
Preparation of azole compounds as PTP1B inhibitors
Ikemoto, Tomoyuki; Tanaka, Masahiro; Yuno, Tako;
Sakamoto, Johei; Nakaniahi, Hiroyuki; Nakagawa,
Yuichi; Ohta, Takeshi; Sakata, Shohei; Morinaga,
Hisayo
CODEN: PIXXD2
PATENT ACC. NUM. COUNT:
1

Apanese
Japanese
Japanese
Japanese
Japanese
Japanese
Japanese

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

	PA'	TENT					DATE							DATE				
	WO	2004															0040	409
		W:	ΑE,	AG,	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
								DE,										
			GE,	GH,	GΜ,	HR,	ΗU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	ĸR,	ΚZ,	LC,
			LK,	LR,	LS,	LT,	LU,	LV,	ΜA,	MD,	MG,	MK,	MN,	MW,	MΧ,	MZ,	NΑ,	NI,
								PL,										
								TZ,										
		RW:						MW,										
								TJ,										
								HU,										
			SK,	TR,	BF,	ΒJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	G₩,	ML,	MR,	ΝE,	SN,
			TD,															
		2004																
	CA	2521	830			AA		2004	1021		CA 2	004-	2521	830		2	0040	409
	EP	1553																
		R:						ES,										
			ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	ΗU,	PL,	SK,
HR																		
	BR	2004	0091	36		Α		2006	0425		BR 2	004-	9136			2	0040	409
	JР	2004 2005 2005 APP	2724	76		A2		2005	1006		JP 2	005-	1337	55		2	0050	428
	NO	2005	0052	46		Α		2005	1221		NO 2	005-	5246			2	0051	108
PRIO	RIT	APP	LN.	INFO	. :						JP 2	003-	1052	67		A 2	0030	409
											JP 2	003-	1575	90	i	A. 2	0030	603
											JP 2	005-	5053	23	i	A3 2	0040	409
											WO 2	004-	JP51	19	,	2	0040	409

OTHER SOURCE(S): MARPAT 141:350161

L19 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

776309-64-9 CAPLUS Glycine, N-[[4-[5-methyl-2-[[4-(1-propy]butyl)phenyl]methoxy]phenyl]-2-thiazolyl]methyl-N-(phenylmethyl)- (SCI) (CA INDEX NAME)

776309-67-2 CAPLUS
Glycine, N-[[4-[5-[1,1-dimethylethyl]-2-[[4-[2-methylpropyl]phenyl]methoxy]phenyl]-2-thiazolyl]methyl]-N-(phenylmethyl)[9CI] (CA INDEX NAME)

776309-76-3 CAPLUS
Glycine, N-{{4-{5-methyl-2-{{4-{1-propylbutyl}phenyl}methoxy}phenyl}-2-thiazolyl]methyl}-N-{2-pyridinylmethyl}- (9CI) (CA INDEX NAME)

L19 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

$$R - \left[L\right] - \left[CH_2\right] - X + \left[CH_2\right] - \left[X + \left[CH_2\right] - X + \left[CH_$$

Title compds. I [V = N, CH; W = S, O; m = 0-2; R1, R2 = H, alkyl; X =

etc.; R4 = H, alkyl; n = 0-4; p = 0, 1; L = CR20R21, etc.; R20 = H,

e.g., prepared from 4-bromoacetylbenzoic acid in 5 steps, followed by saponification
afforded compound II [3-carboxypyridin-5-yloxy] in 44.1% overall yield.

In

PTP1B (protein tyrosine phosphatase 1B) inhibition assays, the IC50 value of compound II [Q = 3-carboxypyridin-5-yloxy] was 0.28 μ M. Compds. I are

claimed useful for the treatment of obesity, diabetes, etc. Formulations

are given. 776309-63-8P 776309-64-9P 776309-67-2P 776309-76-3P IT

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of azole compds. as PTP1B inhibitors for treatment of obesity

ity
 and diabetes)
776309-63-8 CAPLUS
Glycine, N-[[4-[5-methyl-2-[[4-(trifluoromethyl)phenyl]methoxy]phenyl]-2thiazolyl]methyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

L19 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

REFERENCE COUNT:

THERE ARE 16 CITED REFERENCES AVAILABLE FOR

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L19 ANSWER 4 OF 5
ACCESSION NUMBER:
DOCUMENT NUMBER:
1993:671691 CAPLUS
119:271691
1992:671691 CAPLUS
119:271691
1993:671691 CAPLUS
119:271691
Synthesis and antitrypanosomal evaluation of some thiazole-containing amino acids and peptides
AUTHOR(S):
Van Bogaert, I.; Haemets, A.; Bollaert, W.; Van Heirvenne, N.; Brun, R.; Smith, K.; Fairlamb, A. H
Dep. Pharm. Chem., Univ. Antwerp, Antwerp, B-2610, Belg.
SOURCE:
28(5).

387-97 CODEN: EJMCA5; ISSN: 0223-5234 Journal English CASREACT 119:271691

DOCUMENT TYPE: LANGUAGE: OTHER SOURCE(S): GI

AB Several amino acids and peptides containing threates the serious were prepared Thiazole-containing amino acids and peptides I (R1 = H, R2 = H, C02H, Ph; R1 = C02H, CH2C02H, Me, Ph, o-MeOC6H4, m-MeOC6H4, p-MeOC6H4, p-C1C6H4, m-O2NC6H4, p-O2NC6H4, CO-Gly-OH, R2 = H), II, III and IV (R1 = OEt, Gly-OEt) were prepared These compds. were tested in vivo and in vitro

as possible antitrypanosomal agents. Some derivs, showed a slight activity. As they are structurally related to glutathione, their inhibitory properties towards glutathionylspermidine synthetase, trypanothione synthetase and trypanothione reductase were determined No inhibitory activity was found.

150715-80-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
150715-80-3 CAPLUS
2-Thiazolebutanoic acid, α-amino-4-(2-methoxyphenyl)- (9CI) (CA INDEX NAME) IT

L19 ANSWER 5 OF 5
ACCESSION NUMBER:
DOCUMENT NUMBER:
11991:101982 CAPLUS
114:101982
Preparation of heterocyclic guanidines as 5HT3
antagonists
Nagel, Arthur A.; Rizzi, James P.; Rosen, Terry J.
PATENT ASSIGNEE(S):
SOURCE:
DOCUMENT TYPP:
DOCUMENT TYPP:

CAPACITY
DATE:

CAPACITY
DOCUMENT TYPP:

CAPACITY
DATE:

CAPACITY

DOCUMENT TYPE: LANGUAGE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

APPLICATION NO. PATENT NO. KIND DATE DATE US 4963689 EP 397364 EP 397364 R: AT, BE, CH, AT 92062 ES 2058795 IL 94254 CA 2016182 AU 9054767 AU 9054767 A Al Bl 19901016 US 1989-349189 EP 1990-304684 19890509 19901114 19930728 19930728 , ES, FR, 19930815 19941101 19940530 19901109 19960312 GB, GR, IT, LI, LU, NL, SE AT 1990-304684 1 ES 1990-304684 1 IL 1990-94254 1 CA 1990-2016182 DE, DK, E T3 A1 AA C A1 B2 A A A A2 B4 A2 19900430 19900507 19901115 19910926 19901112 AU 1990-54767 19900507 AU 9054767 AU 615385 NO 9002029 ZA 9003478 JP 03011070 JP 06035454 NO 1990-2029 2A 1990-3478 JP 1990-119635 19900508 19900508 19900509 19911224 19910118 HU 58063 PRIORITY APPLN. INFO.: 19920128 HU 1990-2976 US 1989-349189 19900509 A 19890509 EP 1990-304684 A 19900430

OTHER SOURCE(S):

CASREACT 114:101982; MARPAT 114:101982

AHC1 III

Ar-Het-Ch2NR1C(:NR2)NHR3 (I; Ar = naphthyl, indol-3-yl, 2-methylindol-3-yl, 1-methylindol-3-yl, 1-benzylindol-3-ylphenyl, mono-or disubstituted Ph: Het = 4-thiazol-2-yl, 3-isoxazol-5-yl, 2-thien-5-yl, 2-fur-5-yl; Rl = H, Me; R2, R3 = H, hydroxyalkyl, alkyl, cycloalkyl,

; or R2R3 = C2,3 alkylene), useful for treatment of nausea, anxiety, pain, schizophrenia, and gastrointestinal disorders (no data), are prepared

a solution of 3-(chloroacetyl)indole and AcNHCH2C(S)NH2 in EtOH was refluxed

overnight to give 51% 2-(N-acetylaminomethyl)-4-(indol-3-yl)thiazole which

L19 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

- L19 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) was hydrolyzed with concd. Hcl under reflux to give 67% 2-(aminomethyl)-4-(indol-3-yl)thiazole RCl (II). A mixt. of II, 2-methyl-2-thiopseudourea sulfate, and AcONa in isopropanol was heated to reflux overnight to give 83% thiazole salt III. Addnl. 25 I were prepd. IT 132284-03-69 132254-03-6P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as serotoninergic S3 antagonist) 132254-03-6 CAPLUS Guanidine, [[4-(2-methoxyphenyl)-2-thiazolyl]methyl]- (9CI) (CA INDEX NAME)

=> fil reg COST IN U.S. DOLLARS SINCE FILE TOTAL SESSION ENTRY FULL ESTIMATED COST 26.01 707.17 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -3.75 -18.00

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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* The CA roles and document type information have been removed from *

* the IDE default display format and the ED field has been added.

chain nodes : 6 7 8 16 17 18 19 20 23 24 25 27 28 29 32 ring nodes : 1 2 3 4 5 10 11 12 13 14 15 chain bonds : 2-6 3-15 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28 8-29 10-20 11-19 12-16 13-17 14-18 ring bonds : 1-2 1-5 2-3 3-4 4-5 10-11 10-15 11-12 12-13 13-14 exact/norm bonds : 1-2 1-5 2-3 2-6 4-5 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28

chain nodes : 6 7 8 16 17 18 19 20 23 24 25 27 28 29 32 ring nodes : 1 2 3 4 5 10 11 12 13 14 15 chain bonds : 2-6 3-15 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28 8-29 10-20 11-19 12-16 13-17 14-18 ring bonds : 1-2 1-5 2-3 3-4 10-11 10-15 11-12 4 - 5 12-13 13-14 14-15 exact/norm bonds : 4-5 5-32 6-7 6-23 6-24 1-2 1-5 2-3 2-6 7-27 8-28

=> fil caplus COST IN U.S. DOLLARS SINCE FILE TOTAL SESSION ENTRY FULL ESTIMATED COST 1049.77 342.60 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -18.00 0.00

FILE 'CAPLUS' ENTERED AT 08:58:14 ON 24 MAY 2006
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FILE COVERS 1907 - 24 May 2006 VOL 144 ISS 22 FILE LAST UPDATED: 23 May 2006 (20060523/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

L27 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:990095 CAPLUS
DOCUMENT NUMBER: 141:407228
141:407228
3-(Acylamino)salicylamide derivatives and agricultural

fungicides containing them
Hars, Yoshihiko; Kishimoto, Takashi; Sano, Hiroshi;
Haramoto, Hasanori
Hippon Soda Co., Ltd., Japan
Jpn. Kokai Tokkyo Koho, 36 pp.
CODEN: JKXXAP
Patent
Japansee
1 INVENTOR (S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

KIND DATE APPLICATION NO. DATE JP 2004323516 PRIORITY APPLN. INFO.: A2 20041118 JP 2004-112755 JP 2003-107451 20040407 A 20030411

OTHER SOURCE(S): MARPAT 141:407228

The derivs I [R1 = H, C1-6 alkyl; R2 = H, C1-6 alkoxy-C1-6 alkyl, C1-6alkoxycarbonyl, C1-6 alkylcarbonyl, phenyl-C1-8 alkyl; R3 = C1-12 alkyl, C2-8 alkenyl, C2-8 alkynyl, C1-8 haloalkyl, Ph which may be substituted with G, phenyl-C1-8 alkyl which may be substituted with G; R4 = H, C1-6 alkyl; A = Q, Q1 (X = O, S; R5-R6 = C1-8 alkyl, C2-8 alkenyl, C2-8 alkynyl, C1-8 haloalkyl, Ph which may be substituted with G, phenyl-C1-8 alkyl which may be substituted with G, phenyl-C1-8 alkyl which may be substituted with G; R5 and R6 may be ed

ed together to form a ring); G = halo, Cl-6 alkyl, Cl-6 alkoxy, Cl1-6 alkylthio, Cl-6 haloalkyl, Cl-6 haloalkoxyl are useful as agricultural fungicides. Thus, N-[1-(4-methyl-5-phenyloxazol-2-yl)-2-phenylethyl]-3-formamido-2-hydroxybenzamide (preparation given) showed ≥75% control against apple black spot disease due to Venturia inaequalis.

792922-60-2

RI: AGR (Agricultural use); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses) (preparation of N-(heterocyclylmethyl)-3-(acylamino)salicylamides as agrochem. fungicides)

L27 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:101147 CAPLUS
DOCUMENT NUMBER: 140:146128
INVENTOR(S): Freparation of aminosalicylamide derivatives as fungicides
INVENTOR(S): Haramoto, Masahiro
Nippon Soda Co., Ltd., Japan
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan
POCUMENT TYPE: CODEN: PIXXD2
DOCUMENT TYPE: 24bnt Japan
PATENT INFORMATION: 12panese
FAMILY ACC. NUM. COUNT: 12panese

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PA'	TENT	NO.					DATE									ATE	
WO.	2004	10114					2004				003-						-
		AE,															
							DK.										
							IN,										
							MD.										
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	RW:	GH,													AM,	AZ,	BY,
		KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
		FI,	FR,	GB,	GR,	ΗU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
							CM,										
AU	2003	32547	81		A1		2004	0216	- 2	AU 2	003-	2547	81		2	0030	730
PRIORIT	Y APE	LN.	INFO	. :						JP 2	002-	2225	35	1	A 2	0020	731
									,	WO 2	003-	TP96	39		7 2	0030	730

MARPAT 140:146128

Title compds. I and II (Rl, R3 = H, alkyl; R2 = H, alkoxycarbonyl, alkylcarbonyl, phenylalkyl; R4 = alkyl, alkenyl, alkynyl, haloalkyl, Ph, substituted Ph, phenylalkyl; B = Ph, alkyl, alkenyl, alkynyl; X = O, S), useful as fungicides, are prepared Thus, N-[1-{5-phenyloxazol-2-yl}-2,2-

L27 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Cont RN 792922-60-2 CAPLUS CN Benzamide, 3-(formylamino)-2-hydroxy-N-[1-[5-(3-methoxyphenyl)-4-methyl-2-thiazolyl]-2-phenylethyl]- (9CI) (CA INDEX NAME) (Continued)

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) dimethylpropyl]-3-formamido-2-hydroxybenzamide was prepd. and showed fungicidal activity against Venturia inaequalis at 200 ppm. 652152-05-1p

BRI: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation);

USES

(Uses) (Uses)
(preparation of aminosalicylamide derivs. as fungicides)
652152-05-1 CAPIUS
Benzamide, 3-(formylamino)-2-hydroxy-N-(1-[5-(3-methoxyphenyl)-2-thiazolyl)-2-phenylethyl]- (9CI) (CA INDEX NAME)

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

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STRUCTURE FILE UPDATES: 23 MAY 2006 HIGHEST RN 885357-09-5 DICTIONARY FILE UPDATES: 23 MAY 2006 HIGHEST RN 885357-09-5

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* The CA roles and document type information have been removed from *

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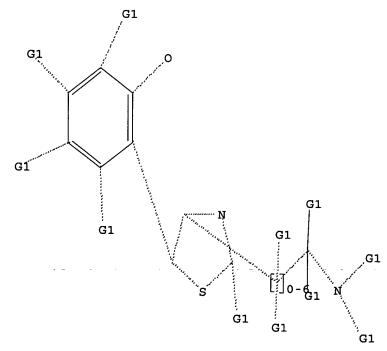
chain nodes : $6 \quad 7 \quad 8 \quad 16 \quad 17 \quad 18 \quad 19 \quad 20 \quad 23 \quad 24 \quad 25 \quad 27 \quad 28 \quad 29 \quad 32$ ring nodes : 1 2 3 4 5 10 11 12 13 14 15 chain bonds : 2-6 3-15 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28 8-29 10-20 11-19 12-16 13-17 14-18 ring bonds : 1-2 1-5 2-3 3-4 4-5 10-11 10-15 11-12 12-13 13-14 exact/norm bonds : 7-8 1-2 1-5 2-3 2-6 4 - 5 5-32 6-7 6-23 6-24 7-27 8-28

chain nodes : $6 \quad 7 \quad 8 \quad 16 \quad 17 \quad 18 \quad 19 \quad 20 \quad 23 \quad 24 \quad 25 \quad 27 \quad 28 \quad 29 \quad 32$ ring nodes : 1 2 3 4 5 10 11 12 13 14 15 chain bonds : 2-6 3-15 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28 8-29 10-20 11-19 12-16 13-17 14-18 ring bonds : 1-2 1-5 2-3 3-4 4-5 10-11 10-15 11-12 12-13 13-14 14-15 exact/norm bonds : 1-2 1-5 2-3 2-6 3-15 5-32 7-25 7-27 8-28 6-23 6-24

chain nodes : 6 7 8 16 17 18 19 20 23 24 25 27 28 29 32 ring nodes : 1 2 3 4 5 10 11 12 13 14 15 chain bonds : 2-6 3-15 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28 8-29 10-20 11-19 12-16 13-17 14-18 ring bonds : 1-2 1-5 2-3 3-4 10-11 10-15 4-5 11-12 12-13 13-14 14-15 exact/norm bonds : 6-7 6-23 1-2 1-5 2-3 2-6 4 - 5 5-32 6-24 7-8 7-25 7-27 8-28

 $\begin{array}{c} G_1 \\ G_2 \\ G_3 \\ G_4 \\ G_4 \\ G_5 \\ G_6 \\ G_6 \\ G_7 \\ G_8 \\$

chain nodes : 6 7 8 16 17 18 19 20 23 24 25 27 28 29 32 ring nodes : 1 2 3 4 5 10 11 12 13 14 15 chain bonds : 2-6·3-15 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28 8-29 10-20 11-19 12-16 13-17 14-18 ring bonds : 1-2 1-5 2-3 3-4 4-5 10-11 10-15 11-12 12-13 13-14 exact/norm bonds : 7-25 7-27 8-28 1-2 1-5 2-3 2-6 5-32 6-7 6-23 6-24 7 - 8



chain nodes : 6 7 8 16 17 18 19 20 23 24 25 27 28 29 32 ring nodes : 1 2 3 4 5 10 11 12 13 14 15 chain bonds : 2-6 3-15 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28 8-29 10-20 11-19 12-16 13-17 14-18 ring bonds : 1-2 1-5 2-3 3-4 4-5 10-11 10-15 11-12 12-13 13-14 exact/norm bonds : 1-2 1-5 2-3 2-6 3-15 4 - 5 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28

chain nodes : 6 7 8 16 17 18 19 20 23 24 25 27 28 29 32 ring nodes : 1 2 3 4 5 10 11 12 13 14 15 chain bonds : 2-6 3-15 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28 8-29 10-20 11-19 12-16 13-17 14-18 ring bonds : 1-2 1-5 2-3 3-4 4-5 10-11 10-15 11-12 12-13 13-14 14-15 exact/norm bonds : 1-2 1-5 2-3 2-6 3-15 4 - 5 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28

```
chain nodes:
6 7 8 16 17 18 19 20 23 24 25 27 28 29 32
ring nodes:
1 2 3 4 5 10 11 12 13 14 15
chain bonds:
2-6 3-15 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28 8-29 10-20 11-19 12-16
13-17 14-18
ring bonds:
1-2 1-5 2-3 3-4 4-5 10-11 10-15 11-12 12-13 13-14 14-15
exact/norm bonds:
1-2 1-5 2-3 2-6 3-4 3-15 4-5 5-32 6-7 6-23 6-24 7-8 7-25 7-27 8-28
```

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BABS - BEILSTEIN Abstracts 1980-present
- BEILSTEIN File of Organic Compounds

CROPR - Derwent Crop Protection Registry

CROPU - DERWENT CROP PROTECTION FILE 1985 - 2003

CSCHEM - ChemSources - USA and International (Chemicals)

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CSNB - Chemical Safety News Base from 1981-present
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DDFU - Derwent Drug File from 1983 - present

DETHERM - DETHERM-DECHEMA thermophysical property database

DGENE - Derwent Geneseq Database 1981 - present
DISSABS - Dissertation Abstracts from 1861 to present

DJSMDS - Derwent Reaction Search Service DJSM (Subscribers)

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DKF - The German Automotive Engineering Database 1974-date

DPCI - Derwent Patents Citation Index 1978 to present

DRUGB - Derwent Drug File, Backfile 1964 - 1982 (Subscribers)
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EPFULL - European Patents Fulltext database
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- IMS LifeCycle, Patent Focus with Patent Family Data
IMSPATENTS
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             - The CAS Patent Markush Learning File
             - The MEDLINE Learning File
LMEDLINE
             - The PATDPA Learning File
LPATDPA
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- Derwent World Patents Index Learning File - The CAS Patent Markush File 1988-present

- The Registry Learning File.

LREGISTRY LWPI

MARPAT

PROMT - PROMT from 1978 - present

PROUSDDR - Drug Data Report from Prous Science

PS - Pharmaceutical Substances

RAPRA - Rubber, Plastics, Polymer Composites 1972 - present

RDISCLOSURE - Research Disclosure 1960 to the present REGISTRY - The CAS Registry File of substances

RSWB - Regional planning and building construction
RTECS - Registry of Toxic Effects of Chemical Substances
RUSSIAPAT - RUSSIAN PATENT ABSTRACTS DATABASE FROM 1994 - PRESENT

SCISEARCH - ISI Science Citation Index from 1974 - present

SOLIDSTATE - Solid State and Superconductivity Abstracts from 1981
SOLIS - German literature in social sciences 1945-present

SOLIS - German literature in social sciences 1945-present SPECINFO - Spectral Database Information System

STNGUIDE - Descriptive information about STN databases

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SYNTHLINE - Synthline Drug Synthesis Database 1984-present
TEMA - TEMA: Technology and Management 1990 to the present
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TOXCENTER - Toxicology Center from 1907 - present

TRIBO - TRIBOLOGY INDEX (Friction, Wear, Lubrication) 1972-pres.

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ULIDAT - Environmental Literature from 1976-present

USAN - USAN - United States Adopted Names

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*** FILE CONTAINS 9,516,393 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

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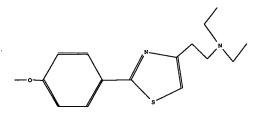
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*

L49 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN

Beilstein Records (BRN): 533129
Beilstein Pref. RN (BPR): 100576-42-9
CAS Reg. NO. (RN): 100576-42-9
Chemical Name (CN):
diethyl-<2-<2-(4-methoxy-phenyl)-thiazol-4yl>-ethyl>-amine

diethyl-<2-<2-(4-methoay-punAutonom Name (AUN):
diethyl-<2-<2-(4-methoxy-phenyl)-thiazol-4yl)-ethyl)-amine
Molec. Formula (MF):
Molecular Weight (MW):
Lawson Number (LN):
Compound Type (CTYPE):
Constitution ID (CONSID):
diethyl-constitution ID (CONSID):
diethyl-constitution (BSO):
Beilstein Citation (BSO):
Entry Date (DED):
1988/11/28
1993/11/23



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
DED	Entry Date	1
DUPD	Update Date	1
CDER	Chemical Derivative	1

L49 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN (Continued) No. of React. Details (.NVAR): 1

Reaction Details:

Reaction RID (.RID): 890695.1
Reaction Classification (.CL): Preparation ethanol Temperature (.T): 60 Cel Reference(a):

REIEFENCE(8):
1. Palazzo,G.; Tavella,M., Gazz.Chim.Ital., CODEN: GCITA9, 92, <1962>, 1084-1092

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L49 ANSWER 1 OF 1 BEILSTEIN COPYRIGHT 2006 BEILSTEIN MDL on STN (Continued)
                                                                                                     1
          PHARM
                           Pharmacological Data
      This substance also occurs in Reaction Documents:
         Code
                                                                                      Occurrence
                           Reaction Documents
Substance is Reaction Product
          RXPRO
 Chemical Derivative:
Derivative BRN (.BRN): 4854668
Reference(s):

1. Palazzo,G.; Tavella,M., Gazz.Chim.Ital., CODEN: GCITA9, 92, <1962>, 1084-1092
Pharmacological Data:
PHARM
Note(s) (.COM): Pharmakol. Wrkg.
Reference(s):
1. Palazzo,G.: Tavella,M., Gazz.Chim.Ital., CODEN: GCITA9, 92, <1962>,
1084-1092
                                                                 1284887
1076118, 605268
4-(2-chloro-ethyl)-2-(4-methoxy-phenyl)-
thiazole, diethylamine
533129
         Reaction ID (.ID):
Reactant BRN (.RBRN):
Reactant (.RCT):
Product BRN (.PBRN): 533129
Product (.PRO): 618thyl-<2-<2-(4-methoxy-phenyl)-thiazol-4-yl>-ethyl>-amine
No. of React. Details (.NVAR): 1
Reaction Details:
         Reaction RID (.RID): 1284887.1
Reaction Classification (.CL): Preparation
Solvent (.SOL): xylene
Temperature (.T): 140 Cel
Reference(s): 1. Palazzo,G.; Tavella,M., Gazz.Chim.Ital., CODEN: GCITA9, 92, <1962>, 1084-1092
Reaction:
RX
                                                                 890695
1072444, 3693764
4-methoxy-thiobenzamide,
1-bromo-4-diethylamino-butan-2-one;
hydrobromide
533129
         Reaction ID (.ID):
Reactant BRN (.RBRN):
Reactant (.RCT):
Product BRN (.PBRN): 533129
Product (.PRO):
diethyl-<2-<2-(4-methoxy-phenyl)-thiazol-4-
yl>-ethyl>-amine
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FULL ESTIMATED COST ENTRY SESSION 40.06 2271.73

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